

Complex Balanced Equilibria of Weakly Reversible Poly-PL Systems: Existence, Stability, and Robustness

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Abstract

Poly-PL kinetic systems (PYK) are kinetic systems consisting of nonnegative linear combinations of power law functions. In this contribution, we analyze these kinetic systems using two main approaches: (1) we define a canonical power law representation of a poly-PL system, and (2) we transform a poly-PL system into a dynamically equivalent power law kinetic system that preserves the stoichiometric subspace of the system. These approaches led us to establish results that concern important dynamical properties of poly-PL systems that extend known results for generalized mass actions systems (GMAS) such as existence, uniqueness and parametrization of complex balanced steady states, and linear stability of complex balanced equilibria. Furthermore, the paper discusses subsets of poly-PL systems that exhibit two types of concentration robustness in some species namely absolute concentration robustness and balanced concentration robustness.

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1 Introduction

Poly-PL kinetic systems (denoted as PYK systems) are kinetic systems formed by nonnegative linear combinations of power law functions. These were introduced by Talabis et al. [26] and were shown to have complex balanced equilibria for weakly reversible such systems with zero kinetic reactant deficiency (called PY-TIK systems). A subset of poly-PL kinetic systems consisting of polynomial kinetics occurs in realizations of evolutionary games as chemical kinetic systems as proposed by Veloz et al. [28], particularly for multi-player games with replicator dynamics. In addition, poly-PL kinetics can be used to study Hill-type kinetics, which include the widely used Michaelis-Menten models, as discussed in [14].

In this contribution, we investigate some important dynamical properties of poly-PL kinetics systems such as existence and parametrization of complex balanced steady states, capacity for multiple complex balanced steady states in a stoichiometric compatibility class, concentration robustness of some species, and linear stability of complex balanced equilibria. The primary approach is to specify power law representations of poly-PL kinetic systems in order to apply or mimic existing results on power law systems. Two approaches are considered in this study: the *canonical PL-representation* and the *STAR-MS transformation* [19] of the poly-PL system (Section 3).

The main contribution of this paper are the following:

- *Section 3:* The results of Müller and Regensburger [21,22] for generalized mass action systems (GMAS) are extended to poly-PL systems. In particular, this work presents partial extensions of the GMAS results to a subset of poly-PL kinetics that are reactant-determined (denoted by PY-RDK systems) and full analogue results for PY-RDK systems with equilibria sets called PL-equilibria and PL-complex balanced equilibria.
- *Section 4:* The set of weakly reversible poly-PL systems with zero kinetic reactant deficiency are shown to be PL-complex balanced.
- *Section 5:* Extensions of the results of Boros et al. [3] on linear

stability of complex balanced equilibria to poly-PL systems are also obtained.

- *Section 6:* Analogues of the results of Fortun and Mendoza [8] involving *absolute concentration robustness* (ACR) and Lao et al. [18] on *balanced concentration robustness* (BCR) for power law kinetic systems to poly-PL kinetic systems are established. Sufficient conditions for concentration robustness in higher deficiency systems are also derived (Section 6.2).

2 Fundamentals of chemical reaction networks and kinetic systems

We denote by \mathbb{R} and \mathbb{Z} the set of real numbers and integers, respectively. For integers a and b , let $\overline{a, b} = \{j \in \mathbb{Z} | a \leq j \leq b\}$. We denote the non-negative real numbers by $\mathbb{R}_{\geq 0}$, and the positive real numbers by $\mathbb{R}_{> 0}$. The sets $\mathbb{R}_{\geq 0}^p$ and $\mathbb{R}_{> 0}^p$ are called the *non-negative* and *positive orthants* of \mathbb{R}^p , respectively. For $x \in \mathbb{R}^p$, the i th coordinate of x is denoted by x_i , where $i \in \overline{1, p}$. The *standard basis* for \mathbb{R}^p is the set $\{\omega_i \in \mathbb{R}^p | i \in \overline{1, p}\}$ and for each $x \in \mathbb{R}^p$ we have the representation $x = \sum_{i=1}^p x_i \omega_i$. Finally, for a vector space V , if S is a non-empty subset of V , the span of S is denoted by $\langle S \rangle$.

2.1 Chemical reaction networks basics

A chemical reaction network (CRN) is a system of interdependent chemical reactions. Each reaction is represented as an ordered pair of vectors, called complexes, of chemical species.

Definition 1. A **chemical reaction network** (CRN) \mathcal{N} is a triple $(\mathcal{S}, \mathcal{C}, \mathcal{R})$ of three finite sets: (1) a set $\mathcal{S} = \{X_1, X_2, \dots, X_m\}$ of **species**, (2) a set \mathcal{C} of **complexes**, consisting of nonnegative linear combinations of the species, and (3) a set $\mathcal{R} = \{R_1, R_2, \dots, R_r\} \subset \mathcal{C} \times \mathcal{C}$ of **reactions** such that $(y, y) \notin \mathcal{R}$ for any $y \in \mathcal{C}$, and for each $y \in \mathcal{C}$, there exists

$y' \in \mathcal{C}$ such that either $(y, y') \in \mathcal{R}$ or $(y', y) \in \mathcal{R}$. We denote the number of species by m , the number of complexes with n and the number of reactions by r .

Alternatively, a CRN can be defined as a directed graph whose vertices are embedded as vectors with nonnegative coefficients in a finite dimensional Euclidean space. In this perspective, the vertices correspond to the complexes and the arcs to the reactions. The species can be identified with the standard unit vectors of the Euclidean space. We assume, as is usual in the literature, that i) each species occurs in at least one complex and ii) each complex occurs in at least one reaction.

We use the convention that an element $(y, y') \in \mathcal{R}$ is denoted by $y \rightarrow y'$. In this reaction, we say that y is the **reactant** complex and y' is the **product** complex. Connected components of a CRN are called **linkage classes**, strongly connected components are called **strong linkage classes**, and strongly connected components without outgoing arcs are called **terminal strong linkage classes**. We denote the number of linkage classes by ℓ , that of the strong linkage classes with $s\ell$, and that of terminal strong linkage classes with t . A complex is called **terminal** if it belongs to a terminal strong linkage class. Otherwise, the complex is called **nonterminal**. A CRN is **weakly reversible** if $s\ell = \ell$ (i.e., every linkage class is a strong linkage class) and **t-minimal** if $t = \ell$ (i.e., every linkage class has one terminal strong linkage class). A CRN is **cycle terminal** if $n_r = n$. A CRN is **cyclic** if it has at least one directed path that starts and ends in the same complex.

With each reaction $y \rightarrow y'$, we associate a **reaction vector** obtained by subtracting the reactant complex y from the product complex y' . The **stoichiometric subspace** S of a CRN is the linear subspace of \mathbb{R}^m defined by $S := \text{span} \{y' - y \in \mathbb{R}^m \mid y \rightarrow y' \in \mathcal{R}\}$. The **rank** of the CRN is defined as $s := \dim S$. Furthermore, if $c \in \mathbb{R}_{\geq 0}^m$, the corresponding **stoichiometric compatibility class** is defined as the intersection of the coset $c + S$ with $\mathbb{R}_{\geq 0}^m$. Two elements a, b of \mathbb{R}^m are **stoichiometrically compatible** if $a - b$ is contained in S . The **deficiency** of a CRN is the nonnegative integer defined by $\delta = n - \ell - s$.

Definition 2. Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a CRN. The **map of complexes** $Y : \mathbb{R}^{\mathcal{C}} \rightarrow \mathbb{R}_{\geq 0}^{\mathcal{S}}$ maps the basis vector ω_y to the complex $y \in \mathcal{C}$. The **incidence map** $I_a : \mathbb{R}^{\mathcal{R}} \rightarrow \mathbb{R}^{\mathcal{C}}$ is the linear map defined by mapping for each reaction $R_j : y_j \rightarrow y'_j \in \mathcal{R}$, the basis vector ω_j to the vector $\omega_{y'_j} - \omega_{y_j} \in \mathcal{C}$. The **stoichiometric map** $N : \mathbb{R}^{\mathcal{R}} \rightarrow \mathbb{R}^{\mathcal{S}}$ is defined as $N = Y \circ I_a$.

2.2 Chemical kinetic system

By *kinetics* of a CRN, we mean the assignment of a rate function to each reaction in the CRN. It is defined formally as follows [29].

Definition 3. A **kinetics** of a CRN $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ is an assignment of a rate function $K_j : \Omega_K \rightarrow \mathbb{R}_{\geq 0}$ to each reaction $R_j \in \mathcal{R}$, where Ω_K is a set such that $\mathbb{R}_{> 0}^m \subseteq \Omega_K \subseteq \mathbb{R}_{\geq 0}^m$. A kinetics for a network \mathcal{N} is denoted by $K = [K_1, K_2, \dots, K_r]^\top : \Omega_K \rightarrow \mathbb{R}_{\geq 0}^r$. The pair (\mathcal{N}, K) is called the **chemical kinetic system (CKS)**.

In this paper, in order to study the dynamics of chemical kinetic systems through systems of ordinary differential equations (ODE), we generally assume that the rate functions are differentiable functions of the variables.

Once a kinetics is associated with a CRN, we can determine the rate at which the concentration of each species evolves at composition $c \in \mathbb{R}_{\geq 0}^m$.

Definition 4. The **species formation rate function** $f : \mathbb{R}_{> 0}^m \rightarrow \mathbb{R}^m$ of a chemical kinetic system (\mathcal{N}, K) is given by

$$f(c) = NK(c) = \sum_{y_j \rightarrow y'_j \in \mathcal{R}} K_j(c)(y'_j - y_j).$$

The equation $dc/dt = f(c)$ is the **ODE or dynamical system** of the CKS. A **positive equilibrium or steady state** c^* is an element of $\mathbb{R}_{> 0}^m$ for which $f(c^*) = 0$. The **set of positive equilibria** of the system is given by $E_+(\mathcal{N}, K) = \{c^* \in \mathbb{R}_{> 0}^m \mid f(c^*) = 0\}$.

A chemical kinetic system is **multistationary** (or has the capacity to admit multiple steady states) if there exist positive rate constants such

that the corresponding ODEs system admits at least two distinct stoichiometrically compatible equilibria. That is, there are at least two positive equilibria belonging to different stoichiometric compatibility class. Otherwise, it is **monostationary**.

The *complex formation rate function* is the analogue of the species formation rate function for complexes.

Definition 5. The **complex formation rate function** $g : \mathbb{R}_{>0}^m \rightarrow \mathbb{R}^n$ of a chemical kinetic system is the given by

$$g(c) = I_a K(c) = \sum_{y_j \rightarrow y'_j \in \mathcal{R}} K_j(c)(\omega_{y'_j} - \omega_{y_j}). \quad (1)$$

Horn and Jackson [16] introduced the notion of *complex balancing* in chemical kinetics, which proved to have profound uses in CRNT. Observe from Equation (1) that the function g gives the difference between the production and degradation of each complex. Thus, “complex balancing” occurs when $g(c) = 0$. A chemical kinetic system (\mathcal{N}, K) is called **complex balanced** if it has a complex balanced steady state. The set of positive complex balanced steady states of the system is given by $Z_+(\mathcal{N}, K) = \{c \in \mathbb{R}_0^m \mid g(c) = 0\}$.

Power law kinetics is defined by an $r \times m$ matrix $F = [F_{ij}]$, called the **kinetic order matrix**, and vector $k \in \mathbb{R}_{>0}^r$, called the **rate vector**.

Definition 6. A kinetics $K : \mathbb{R}_{>0}^m \rightarrow \mathbb{R}^r$ is a **power law kinetics** (PLK) if

$$K_i(x) = k_i x^{F_{i\cdot}}, \quad \text{for all } i \in \overline{1, r},$$

with $k_i \in \mathbb{R}_{>0}$ and $F_{ij} \in \mathbb{R}$. A PLK system has **reactant-determined kinetics** (of type **PL-RDK**) if for any two reactions $R_i, R_j \in \mathcal{R}$ with identical reactant complexes, the corresponding rows of kinetic orders in F are identical, i.e. $F_{ih} = F_{jh}$ for $h \in \overline{1, m}$. Otherwise, a PLK system has **non-reactant-determined kinetics** (of type **PL-NDK**).

An example of PL-RDK is the well-known **mass action kinetics** (MAK), where the kinetic order matrix is the transpose of the map of complexes Y [6].

Arceo et al. [2] identified two large sets of kinetic systems, namely the **complex factorizable** (CF) kinetics and its complement, the **non-complex factorizable** (NF) kinetics. Complex factorizable kinetics generalize the key structural property of MAK that the species formation rate function decomposes as $dx/dt = Y \circ A_k \circ \Psi_K$, where Y is the map of complexes, A_k is the Laplacian map, and $\Psi_K : \mathbb{R}_{\geq 0}^{\mathcal{L}} \rightarrow \mathbb{R}_{\geq 0}^{\mathcal{C}}$ such that $I_a \circ K(x) = A_k \circ \Psi_K(x)$ for all $x \in \mathbb{R}_{\geq 0}^{\mathcal{L}}$. In the set of power law kinetics, the complex-factorizable kinetic systems are precisely the PL-RDK systems.

2.3 Decomposition theory

We refer to [5] for more details on the concepts and results in decomposition theory.

Definition 7. Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a CRN. A **covering** of \mathcal{N} is a collection of subsets $\{\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_p\}$ whose union is \mathcal{R} . A covering is called a **decomposition** of \mathcal{N} if the sets \mathcal{R}_i form a partition of \mathcal{R} .

Each \mathcal{R}_i defines a subnetwork \mathcal{N}_i of \mathcal{N} wherein \mathcal{C}_i consists of all complexes occurring in \mathcal{R}_i and \mathcal{S}_i consists of all the species occurring in \mathcal{C}_i .

Feinberg [7] identified an important class of network decomposition called *independent decomposition*. A decomposition is **independent** if the stoichiometric subspace S of a network is the direct sum of the subnetworks' stoichiometric subspaces S_i or equivalently, if $s = s_1 + s_2 + \dots + s_p$. Fortun et al. [10] derived a basic property of independent decompositions:

Proposition 1. *If $\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2 \cup \dots \cup \mathcal{N}_p$ is an independent decomposition, then $\delta \leq \delta_1 + \delta_2 + \dots + \delta_p$, where δ_i represents the deficiency of the subnetwork \mathcal{N}_i .*

Feinberg [7] established the following relationship between the positive equilibria of the “parent network” and those of the subnetworks of an independent decomposition:

Theorem 2 (Feinberg Decomposition Theorem, [7]). *Let $\{\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_p\}$ be a partition of a CRN \mathcal{N} and let K be a kinetics on \mathcal{N} . If $\mathcal{N} =$*

$\mathcal{N}_1 \cup \mathcal{N}_2 \cup \dots \cup \mathcal{N}_p$ is the network decomposition generated by the partition and $E_+(\mathcal{N}_i, K_i) = \{x \in \mathbb{R}_{\geq 0}^m \mid N_i K_i(x) = 0\}$, then

$$(i) \quad \bigcap_{i \in \overline{1,p}} E_+(\mathcal{N}_i, K_i) \subseteq E_+(\mathcal{N}, K)$$

(ii) If the network decomposition is independent, then equality holds.

Farinas et al. [5] introduced the concept of an *incidence independent decomposition*, which naturally complements the independence property. A decomposition of a CRN \mathcal{N} is **incidence independent** if the image of the incidence map I_a of \mathcal{N} is the direct sum of the images of the incidence maps of the subnetworks. It follows that the dimension of the image of the incidence map I_a equals the sum of the dimensions of the subnetworks' incidence maps. That is, $n - \ell = \sum(n_i - \ell_i)$. The linkage classes form the primary example of an incidence independent decomposition, since $n = \sum n_i$ and $\ell = \sum \ell_i$.

The following result is the analogue of Proposition 1 for incidence independent decomposition.

Proposition 3 (Prop. 7, [5]). *Let $\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2 \cup \dots \cup \mathcal{N}_p$ be an incidence independent decomposition. Then $\delta \geq \delta_1 + \delta_2 + \dots + \delta_p$.*

\mathcal{C} -decompositions form an important class of incidence independent decompositions:

Definition 8. A decomposition $\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2 \cup \dots \cup \mathcal{N}_p$ with $\mathcal{N}_i = (\mathcal{S}_i, \mathcal{C}_i, \mathcal{R}_i)$ is a **\mathcal{C} -decomposition** if $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for $i \neq j$.

A \mathcal{C} -decomposition partitions not only the set of reactions but also the set of complexes. The primary examples of \mathcal{C} -decomposition are the linkage classes.

The following result shows the relationship between the set of incidence independent decompositions and the set of complex balanced equilibria of any kinetic system. It is the precise analogue of Feinberg's result (Theorem 2).

Theorem 4 (Theorem 4, [5]). *Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a CRN and $\mathcal{N}_i = (\mathcal{S}_i, \mathcal{C}_i, \mathcal{R}_i)$ for $i \in \overline{1,p}$ be the subnetworks of a decomposition. Let K be*

any kinetics, and $Z_+(\mathcal{N}, K)$ and $Z_+(\mathcal{N}_i, K_i)$ be the set of complex balanced equilibria of \mathcal{N} and \mathcal{N}_i , respectively. Then

$$(i) \quad \bigcap_{i \in \overline{1, p}} Z_+(\mathcal{N}_i, K_i) \subseteq Z_+(\mathcal{N}, K)$$

If the decomposition is incidence independent, then

$$(ii) \quad Z_+(\mathcal{N}, K) = \bigcap_{i \in \overline{1, p}} Z_+(\mathcal{N}_i, K_i)$$

$$(iii) \quad Z_+(\mathcal{N}, K) \neq \emptyset \text{ implies } Z_+(\mathcal{N}_i, K_i) \neq \emptyset \text{ for each } i \in \overline{1, p}.$$

The converse statement of Theorem 4 (iii) holds for a subset of incidence independent decompositions with any kinetics:

Proposition 5 (Theorem 5, [5]). *Let $\mathcal{N} = \mathcal{N}_1 \cup \mathcal{N}_2 \cup \dots \cup \mathcal{N}_p$ be a weakly reversible \mathcal{C} -decomposition of a chemical kinetic system (\mathcal{N}, K) . If $Z_+(\mathcal{N}_i, K_i) \neq \emptyset$ for each $i \in \overline{1, p}$, then $Z_+(\mathcal{N}, K) \neq \emptyset$.*

3 Complex balanced poly-PL kinetic systems

Poly-PL systems were introduced by Talabis et al. in [26] and applied to study evolutionary games with replicator dynamics and polynomial payoff functions. A computational approach to determine their multistationarity was developed by Magpantay et al. [19]. In this section, we first collect concepts, techniques and results from these papers and then apply them to the extension of the results of Müller and Regensburger on Generalized Mass Action Systems (GMAS) to classes of poly-PL systems.

3.1 Poly-PL systems: canonical PL-representation and STAR-MSC transformation

We recall the definition and introduce some additional notation for a PY-RDK system from Talabis et al. [26]:

Definition 9. A kinetics $K : \mathbb{R}_{>0}^m \rightarrow \mathbb{R}^r$ is a **poly-PL kinetics** if

$$K_i(x) = k_i (a_{i,1}x^{F_{i,1}} + a_{i,2}x^{F_{i,2}} + \cdots + a_{i,h_i}x^{F_{i,h_i}}) \quad \text{for } i \in \overline{1, r} \quad (2)$$

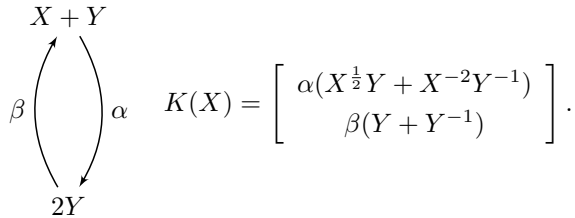
written in lexicographic order with $k_i \in \mathbb{R}_{>0}$, $a_{i,j} \in \mathbb{R}_{\geq 0}$, $F_{i,j} \in \mathbb{R}^m$, and $j \in \overline{1, h_i}$ (where h_i is the number of terms in reaction i). Power-law kinetics is defined by the $r \times m$ **kinetic order matrices** $[F_{i,j}]$, the **rate vector** $[k_i] \in \mathbb{R}_{>0}^r$, and the **poly-rate vectors** $[a_{i,j}] \in \mathbb{R}_{>0}^r$. If $h = \max h_i$, we normalize the length of each kinetics to h by replacing the last term with $(h - h_i + 1)$ terms with $\frac{1}{h-h_i+1}x^{F_{i,h_i}}$. We call this the **canonical representation** of a poly-PL kinetics.

Henceforth, for each $j \in \overline{1, h}$, we set $\mathcal{K}_j(x) := k_i a_{i,j} x^{F_{i,j}}$ where $i \in \overline{1, r}$. Furthermore, we use the notation $\{\mathcal{K}_j\}$ (where $j \in \overline{1, h}$) or $K = \mathcal{K}_1 + \mathcal{K}_2 + \cdots + \mathcal{K}_h$ to denote the PL-representation of a poly-PL kinetics.

Running Example - Part 1. Consider the ODE system:

$$\begin{aligned} \dot{X} &= -\alpha(X^{\frac{1}{2}}Y + X^{-2}Y^{-1}) + \beta(Y + Y^{-1}) \\ \dot{Y} &= \alpha(X^{\frac{1}{2}}Y + X^{-2}Y^{-1}) - \beta(Y + Y^{-1}) \end{aligned}$$

The corresponding weakly reversible network and kinetics will be



The kinetic order matrices, rate vector and poly-rate vectors are given below.

$$F_1 = \begin{bmatrix} \frac{1}{2} & 1 \\ 0 & 1 \end{bmatrix} \quad a_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad F_2 = \begin{bmatrix} -2 & -1 \\ 0 & -1 \end{bmatrix} \quad a_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad k = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}.$$

We extend the definition of PL-RDK kinetics to poly-PL kinetics.

Definition 10. A poly-PL kinetic system (\mathcal{N}, K) is said to be have

reactant-determined kinetics if and only if for each $(\mathcal{N}, \mathcal{K}_j)$ obtained from the PL-representation $\{\mathcal{K}_j\}$ of the system, $(\mathcal{N}, \mathcal{K}_j)$ is PL-RDK and $a_{i,j} = a_{i',j}$ for any two reactions $R_i, R_{i'}$ of a branching node. We denote such poly-PL system by **PY-RDK**.

Running Example - Part 2. The kinetics K in the running example is PY-RDK. The \mathcal{K}_j 's are

$$\mathcal{K}_1(x) = \begin{bmatrix} \alpha X^{1/2} Y \\ \beta Y \end{bmatrix} \quad \mathcal{K}_2(x) = \begin{bmatrix} \alpha X^{-2} Y^{-1} \\ \beta Y^{-1} \end{bmatrix}.$$

Clearly, $K = \mathcal{K}_1 + \mathcal{K}_2$.

The **S-invariant termwise addition of reactions via maximal stoichiometric coefficients (STAR-MSc)** method is based on the idea to use the maximal stoichiometric coefficient (MSC) among the complexes in the CRN to construct reactions whose reactant complexes and product complexes are different from existing ones. This is done by uniform translation of the reactants and products to create a “replica” of the CRN. The method creates $h - 1$ replicas of the original network and hence its transform, \mathcal{N}^* becomes the union (in the sense of [13]) of the replicas and the original CRN.

We now describe the STAR-MSc transformation. Since the domain of definition of a poly-PL kinetics is $\mathbb{R}_{>0}^m$, all $x = (X_1, X_2, \dots, X_m)$ are positive vectors. Let $M = 1 + \max\{y_i \mid y \in \mathcal{C}\}$, where the second summand is the maximal stoichiometric coefficient.

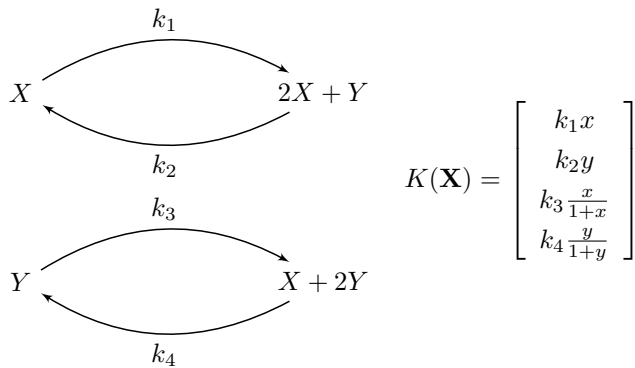
For any positive integer z , define the vector \mathbf{z} to be the vector $(z, z, \dots, z) \in \mathbb{R}^m$. For each complex $y \in \mathcal{C}$, form the $(h - 1)$ complexes

$$y + \underline{M}, y + \underline{2M}, \dots, y + \underline{(h - 1)M}.$$

Each of these complexes are different from each other and from all existing complexes. Further properties of the STAR-MSc transformation are discussed in [19].

Example 1. Consider the following weakly reversible network with two

species X and Y . The kinetics are also given below.



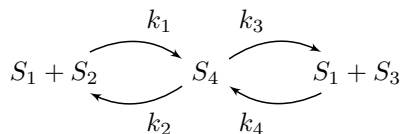
K_3 and K_4 are of Hill type kinetics. Using the transformation of Hernandez and Mendoza [14], the associated kinetics will be a poly-PL kinetics given by:

$$K_{PY}(\mathbf{X}) = \begin{bmatrix} k_1 x(1+x)(1+y) \\ k_2 y(1+x)(1+y) \\ k_3 x(1+y) \\ k_4 y(1+x) \end{bmatrix}.$$

The canonical PL-representation of a poly-PL kinetics is

$$K_{PY}(\mathbf{X}) = \begin{bmatrix} k_1(x + x^2 + xy + x^2y) \\ k_2(y + xy + y^2 + xy^2) \\ k_3(xy + \frac{1}{3}x + \frac{1}{3}x + \frac{1}{3}x) \\ k_4(xy + \frac{1}{3}y + \frac{1}{3}y + \frac{1}{3}y) \end{bmatrix}.$$

Example 2. Consider the following Michaelis-Menten kinetic system from Enzyme biology with set of biochemical species $S = \{S_1, S_2, S_3, S_4\}$, set of complexes $\{S_1 + S_2, S_1 + S_3, S_4\}$, and reactions:



This network assumes the Michaelis–Menten enzyme mechanism, in which a substrate S_2 is modified into a substrate S_3 through the formation of an intermediate S_4 . The reaction is catalyzed by an enzyme S_1 . The kinetic systems associated to the ODE system are:

$$K_{MAK}(\mathbf{X}) = \begin{bmatrix} k_1 S_1 S_2 \\ k_2 S_3 \\ k_3 S_3 = v_f \\ k_4 S_1 S_3 = v_b \end{bmatrix} \quad \text{and} \quad K_{PQK}(\mathbf{X}) = \begin{bmatrix} k_1 S_1 S_2 \\ k_2 S_3 \\ k_1 \frac{S_2}{1+k_3 S_2+S_4} \\ k_2 \frac{S_4}{1+k_3 S_2+S_4} \end{bmatrix}.$$

The kinetics $K_{PQK}(\mathbf{X})$ is taken from the collection of enzymatic reactions in Appendix 2 of [12]. The forward rate v_f and the backward rate v_b are replaced by rational expressions $k_1 \frac{S_2}{1+k_3 S_2+S_4}$ and $k_2 \frac{S_4}{1+k_3 S_2+S_4}$, respectively.

Using the transformation in Section 6.1 of [14], the associated kinetics will be a poly-PL kinetics in the form:

$$K_{PY}(\mathbf{X}) = \begin{bmatrix} k_1(S_1 S_2 + k_3 S_1 S_2^2 + S_1 S_2 S_4) \\ k_2(S_3 + k_3 S_2 S_3 + S_3 S_4) \\ k_1 S_2 \\ k_2 S_4 \end{bmatrix}.$$

The canonical PL-representation of a poly-PL kinetics is

$$K_{PY}(\mathbf{X}) = \begin{bmatrix} k_1(S_1 S_2 + k_3 S_1 S_2^2 + S_1 S_2 S_4) \\ k_2(S_3 + k_3 S_2 S_3 + S_3 S_4) \\ k_1(\frac{1}{3} S_2 + \frac{1}{3} S_2 + \frac{1}{3} S_2) \\ k_2(\frac{1}{3} S_4 + \frac{1}{3} S_4 + \frac{1}{3} S_4) \end{bmatrix}.$$

3.2 Extension of GMAS theory to PY-RDK systems

A kinetics K on a weakly reversible network \mathcal{N} has **conditional complex balancing (CCB)** if there exist rate constants such that (\mathcal{N}, K) is complexed balanced, i.e., $Z_+(\mathcal{N}, K) \neq \emptyset$. A kinetics is **unconditionally complex balanced (UCB)** on a weakly reversible network if for all rate constants, $Z_+(\mathcal{N}, K) \neq \emptyset$.

Poly-PL kinetic systems belong to a large set of chemical kinetics called **rate constant-interaction map decomposable (RID) kinetics**. RID kinetic systems are chemical systems with constant rates [23]. In Appendix A, we define this system formally and we derive the Conditional Complex Balancing (CCB) property for any poly-PL kinetics on a weakly reversible network from a general result on RID kinetics.

We recall, from [22], that a **generalized mass action system (GMAS)** is a 4-tuple (G, y, \tilde{y}, k) where G is a digraph with n vertices and ℓ connected components, y maps the complexes into \mathbb{R}^m , \tilde{y} maps the reactant complexes to \mathbb{R}^m and k is a vector of rate constants. The image of y can be viewed as the (stoichiometric) complexes of a CRN. The image of \tilde{y} is the set of **kinetic complexes**. It was shown in [25] that a PL-RDK system corresponds to a GMAS with an injective map y .

The cornerstone of the theory of Müller-Regensburger for GMAS systems [21] is the concept of kinetic deficiency $\tilde{\delta}$, which in turn is based on the concept of a kinetic order subspace \tilde{S} . The kinetic deficiency is defined as $\tilde{\delta} = n - l - \dim(\tilde{S})$. Recall that for a weakly reversible GMAS system, the kinetic order subspace \tilde{S} is the span $\langle \tilde{y}' - \tilde{y} \rangle$ where \tilde{y}', \tilde{y} are kinetic complexes of $y \rightarrow y'$ in $\mathbb{R}^{\mathcal{S}}$.

We extend the concept of kinetic order subspace to a PY-RDK system as follows: to each reaction, we assign the h -vector of kinetic complexes of $(\mathcal{N}, \mathcal{K}_j)$ in the direct sum of \mathbb{R}^m h -times. Since the system is complex factorizable, this is also map from the set of reactant complexes of \mathcal{N} . We define \tilde{S} as follows:

Definition 11. The **kinetic order subspace** of a poly-PL system is the direct sum $\tilde{S} = \tilde{S}_1 + \cdots + \tilde{S}_h$, considered as a subspace of the direct sum of \mathbb{R}^m h -times. Here, \tilde{S}_j is the kinetic order subspace of the GMAS system $(\mathcal{N}, \mathcal{K}_j)$ (where $j \in \overline{1, h}$). The **dimension** of the kinetic order subspace, \tilde{s}_j , and the **kinetic deficiency**, $\tilde{\delta}$, of the poly-PL system (\mathcal{N}, K) are defined as $\tilde{s} = \tilde{s}_1 + \cdots + \tilde{s}_h$ and $\tilde{\delta} = \tilde{\delta}_1 + \cdots + \tilde{\delta}_h$, respectively. Here, $\tilde{s}_j = \dim \tilde{S}_j$ and $\tilde{\delta}_j = n - l - \tilde{s}_j$ (for each $j \in \overline{1, h}$).

We present partial extensions of the GMAS results to PY-RDK systems. First, we show that zero kinetic deficiency is sufficient for uncondi-

tional complex balancing:

Proposition 6. *Let (\mathcal{N}, K) be a weakly reversible PY-RDK system with $\tilde{\delta} = 0$. Then $Z_+(\mathcal{N}, K) \neq \emptyset$ for any set of rate constants.*

Proof. Let (\mathcal{N}^*, K^*) be the STAR-MSK transform of (\mathcal{N}, K) . Since \mathcal{N} is weakly reversible, each \mathcal{N}_j^* is weakly reversible. Moreover, $\tilde{\delta} = 0$ implies that $\tilde{\delta}_j = 0$. By the GMAS unconditional complex balancing, we have $Z_+(\mathcal{N}, \mathcal{K}_j) \neq \emptyset$ and hence, $Z_+(\mathcal{N}_j^*, K_j^*) \neq \emptyset$. Since these sets form a \mathcal{C} -decomposition of (\mathcal{N}_j^*, K_j^*) , we have $\emptyset \neq Z_+(\mathcal{N}_j^*, K_j^*) = \bigcap Z_+(\mathcal{N}, \mathcal{K}_j)$. Therefore, $Z_+(\mathcal{N}, K) \neq \emptyset$ for any set of rate constants. ■

The poly-PL systems in Examples 1 and 2 are weakly reversible PY-RDK with $\tilde{\delta} = 0$. Hence, these systems are unconditionally complexed balanced. The following corollary illustrates the usefulness of the above extension:

Corollary. *Let (\mathcal{N}, K) be a weakly reversible PY-RDK system. If its canonical PL-representation $\{\mathcal{K}_j\}$ consists of PL-RDK systems with zero kinetic deficiency, then $Z_+(\mathcal{N}, K) \neq \emptyset$ for any set of rate constants.*

The STAR-MSK transform (\mathcal{N}^*, K^*) as a PL-RDK system also has a kinetic deficiency, which we denote by $\tilde{\delta}^*$. We document an interesting relation to $\tilde{\delta}$ as well as two other bounds in the following proposition:

Proposition 7. *Let (\mathcal{N}^*, K^*) be the STAR-MSK transform of (\mathcal{N}, K) . Then*

$$(i) \quad \tilde{\delta}^* \leq h(n - \ell) - 1.$$

$$(ii) \quad \text{If } h \geq m, \text{ then } \tilde{\delta}^* \geq \tilde{\delta}.$$

$$(iii) \quad \text{If } \mathcal{N} \text{ is open (i.e., non-mass conserving), then } \tilde{\delta}^* \geq \delta^*.$$

Proof. For the kinetic rank \tilde{s}^* we have $1 \leq \tilde{s}^* \leq m$. Hence, $h(n - \ell) - m \leq \tilde{\delta}^* \leq h(n - \ell) - 1$, which shows (i). For (ii), note that $h(n - \ell) - m = h(n - \ell) - \tilde{s} + (\tilde{s} - m)$ so that $\tilde{\delta}^* - \tilde{\delta} \geq \tilde{s} - m \geq h - m$, since $\tilde{s}_j \geq 1$. The assumption that $h \geq m$ shows the claim. For (iii), by assumption, $s = m$ and $s = s^*$ so that the claim follows as well. ■

We introduce equilibria subsets to which the full analogues of the parametrization and monostationarity results for GMAS systems can be extended.

Definition 12. The set of **PL-equilibria** $E_{+,PL}(\mathcal{N}, K)$ and of **PL-complex balanced equilibria** $Z_{+,PL}(\mathcal{N}, K)$ of a poly-PL kinetic system are defined as $E_{+,PL}(\mathcal{N}, K) := \bigcap E_+(\mathcal{N}, \mathcal{K}_j)$ and $Z_{+,PL}(\mathcal{N}, K) := \bigcap Z_+(\mathcal{N}, \mathcal{K}_j)$.

A PYK system is called PL-complex balanced if $\emptyset \neq Z_+(\mathcal{N}, K) = Z_{+,PL}(\mathcal{N}, K)$. The next result is the parametrization of a subset of the set of complex balanced equilibria:

Proposition 8. *For any PY-RDK system with complex balanced equilibrium $c^* \in Z_{+,PL}(\mathcal{N}, K)$,*

$$Z_{+,PL}(\mathcal{N}, K) = \{c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in (\tilde{S})^\perp\}. \quad (3)$$

Proof. By assumption, for each $j \in \overline{1, h}$, $c^* \in Z_+(\mathcal{N}, \mathcal{K}_j)$. By GMAS parametrization (Prop. 2.21 of [21]), we have $Z_+(\mathcal{N}, \mathcal{K}_j) = \{c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in (\tilde{S}_j)^\perp\}$. This is equivalent to

$$\begin{aligned} Z_{+,PL}(\mathcal{N}, K) &= \bigcap \left\{ c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in (\tilde{S}_j)^\perp \right\} \\ &= \left\{ c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in \bigcap (\tilde{S}_j)^\perp \right\} \\ &= \left\{ c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in (\tilde{S})^\perp \right\} \text{ since } \bigcap (\tilde{S}_j)^\perp \\ &= \left(\sum \tilde{S}_j \right)^\perp. \quad \blacksquare \end{aligned}$$

Recall that the **sign function** of a real vector assigns to each coordinate either -1 , 1 or 0 depending on whether the coordinate is negative, positive or zero. When applied to a kinetic vector in $\mathbb{R}^m \times \dots \times \mathbb{R}^m$, it can be viewed both as a “long” vector $(\text{sign}_1, \dots, \text{sign}_h)$ or a vector of m -tuples, since the sign function does not depend on the ambient vector space. Finally, we obtain the criterion for monostationarity in a restricted form:

Proposition 9. *A weakly reversible PY-RDK system has at most one complex balanced PL-equilibrium in a stoichiometric class if and only if $\text{sign}(S) \cap \text{sign}(\widetilde{S})^\perp = 0$.*

Proof. We have

$$\text{sign}(\widetilde{S})^\perp = (\text{sign}(\widetilde{S}_1)^\perp, \dots, \text{sign}(\widetilde{S}_h)^\perp) \text{ and } \text{sign}(S) = (\text{sign}(S), \dots, \text{sign}(S)).$$

For the forward implication, let c^* be a PL-equilibrium. It is contained in each $Z_+(\mathcal{N}, \mathcal{K}_j)$ where for each $j \in \overline{1, h}$, the sign conditions hold. This results in the hm 0-vector for the overall sign condition. For the backward direction, if the intersection is the hm 0-vector, we have h m -tupled zero vectors for the intersections of $\text{sign}(S) \cap \text{sign}(\widetilde{S}_j)^\perp$. If we consider S and S_j 's as subspaces of $\text{Im } Y^*$ (i.e. the map of complexes of \mathcal{N}^* in a single \mathbb{R}^m), we can conclude, since the sign values do not change, that (\mathcal{N}^*, K^*) is a weakly reversible PL-RDK system with at most one equilibria in every stoichiometric class. Since $Z_+(\mathcal{N}^*, K^*) = Z_{+, \text{PL}}(\mathcal{N}, K)$ and $S^* = S$, we obtain the claim. ■

Proposition 10. *If a weakly reversible PY-RDK system is PL-complex balanced, i.e., has the property $Z_+(\mathcal{N}, K) = Z_{+, \text{PL}}(\mathcal{N}, K)$, then we have:*

- (i) **Unconditional complex balancing:** $\widetilde{\delta} = 0$ if and only if $Z_+(\mathcal{N}, K) \neq \emptyset$ for any set of rate constants
- (ii) **Parametrization:** $Z_+(\mathcal{N}, K) = \{c \in \mathbb{R}_{>0}^m \mid \ln(c) - \ln(c^*) \in (\widetilde{S})^\perp\}$
- (iii) **Monostationarity criterion:** *The poly-PL kinetic system (\mathcal{N}, K) is monostationary if and only if $\text{sign}(S) \cap \text{sign}(\widetilde{S})^\perp = 0$.*

4 Weakly reversible poly-PL systems with zero kinetic reactant deficiency

In this Section, we present the set PY-TIK of poly-PL systems with zero kinetic reactant deficiency as an interesting example of PL-complex balanced systems with zero kinetic deficiency. We first review briefly the

results in the special case $h = 1$, i.e. power law systems. We then present the Zero Kinetic Reactant Deficiency (ZKRD) Theorem for PY-TIK, from which the PL-complex balancing property of PY-TIK systems follows. We conclude with a discussion of particular aspects of PY-TIK systems arising from the extension of GMAS properties to PL complex balanced systems presented in Section 3.

4.1 A brief review of concepts and results for $h = 1$ (PL-TIK systems)

When studying PL-RDK systems, it is more convenient to use the $m \times n_r$ T-matrix rather than the $r \times m$ kinetic order matrix: $T_{i,\rho(q)} := F_{q,i}^T$, where $i = 1, \dots, m, q = 1, \dots, r$ and ρ is the reactant map. PL-TIK systems were first identified by Talabis et al [25] as a subset of PL-RDK systems whose T matrix columns in each linkage class were linearly independent (PL-LLK, s. Figure 1). Their defining property was the maximal rank of their augmented T-matrix, e.g. the $(m+l) \times n_r$ matrix \hat{T} formed by adding the characteristic function of reactants per linkage class to the T-matrix.

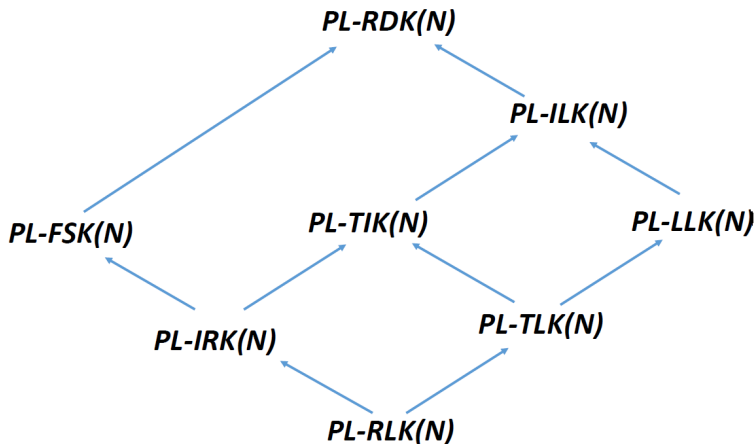


Figure 1. PL-ILK and related kinetic sets

Analogues of the Deficiency Zero Theorem (DZT) and the Deficiency One Theorem (DOT) for mass action systems were derived. While the DZT is a special case of a general result by Müller and Regensburger for GMAS [21], the DOT extension, to our knowledge, remains unique to date. In parallel, Arceo et al [1] studied the relations of reactant subspaces of CRN to kinetics and by introducing the concept of reactant deficiency showed similarities to work on PL-TIK. After a special case was derived as a “Weak Reversibility Theorem” by Mendoza et al [20], the full Zero Kinetic Reactant Deficiency (ZKRD) Theorem was established by Talabis et al [27] where the new characterization of PL-TIK via the concept of kinetic reactant deficiency was introduced.

4.2 The zero kinetic reactant deficiency (ZKRD) theorem for PY-TIK implies PL-complex balancing

Let (\mathcal{N}, K) be a PY-RDK system with canonical PL-representation $K = \mathcal{K}_1 + \dots + \mathcal{K}_h$. We now formally define the kinetic reactant deficiency of (\mathcal{N}, K) .

For each kinetic order matrix F_j ($\forall j \in \overline{1, h}$), we define the $m \times n$ matrix \tilde{Y}_j defined as:

$$(\tilde{Y}_j)_{ij} = \begin{cases} (F_j)_{ri}, & \text{if } j \text{ is a reactant complex of reaction } r \\ 0, & \text{otherwise} \end{cases}$$

Definition 13. The $m \times n_r$ **poly T-matrix** T_j ($\forall j \in \overline{1, h}$) is the truncated \tilde{Y}_j where the non-reactant columns are deleted. Define the $n_r \times l$ matrix $L = [e_1, e_2, \dots, e_l]$ where e^i is a characteristic vector for linkage class \mathcal{L}^i . The block matrix $\hat{T}_j \in \mathbb{R}^{(m+l) \times n_r}$ ($\forall j \in \overline{1, h}$) is defined as

$$\hat{T}_j = \begin{bmatrix} T_j \\ L^\top \end{bmatrix}. \quad (4)$$

Definition 14. The block matrix $\widehat{T} \in \mathbb{R}^{h \cdot (m+l) \times h \cdot n_r}$ is defined as

$$\widehat{T} = \begin{bmatrix} \widehat{T}_1 & & 0 \\ & \ddots & \\ 0 & & \widehat{T}_h \end{bmatrix} \quad (5)$$

Definition 15. Let \mathcal{N} be a network with n_r reactant complexes and K a poly-PL kinetics with poly T-matrices T_1, \dots, T_h . If $\widehat{q} = \text{rank}(\widehat{T})$, then the **kinetic reactant deficiency** $\widehat{\delta}$ is defined as

$$\widehat{\delta} = h \cdot n_r - \widehat{q}. \quad (6)$$

Definition 16. The set PY-TIK consists of all complex factorizable poly-PL kinetics with zero kinetic reactant deficiency.

We have the following basic relationships between the kinetic reactant properties of the PY-TIK system and its PL-representation systems. Note that the block matrices \widehat{T}_j is that of the PLK system $(\mathcal{N}, \mathcal{K}_j)$. Set \widehat{q}_j and $\widehat{\delta}_j$ be its kinetic reactant rank and kinetic reactant deficiency, respectively.

Proposition 11. *Let (\mathcal{N}, K) be a poly-PL system with canonical PL-representation $K = \mathcal{K}_1 + \dots + \mathcal{K}_h$. Then*

$$(i) \quad \widehat{\delta} = \widehat{\delta}_1 + \dots + \widehat{\delta}_h;$$

(ii) (\mathcal{N}, K) is PY-TIK if and only if each $(\mathcal{N}, \mathcal{K}_j)$ is PL-TIK.

Proof. (i) follows directly from the definition of the block matrix \widehat{T} as direct sum of the \widehat{T}_j , which implies $\widehat{\delta} = \widehat{\delta}_1 + \dots + \widehat{\delta}_h$. (ii) follows from (i) directly, too. ■

We recall from [26] the complex equilibria existence parametrization and uniqueness statements of the Zero Kinetic Reactant Deficiency (ZRKD) Theorem for PY-TIK:

Theorem 12. *Let (\mathcal{N}, K) be a PY-TIK systems, that is, (\mathcal{N}, K) has a complex factorizable kinetics and $\widehat{\delta} = 0$. Then \mathcal{N} is weakly reversible if and only if $Z_+(\mathcal{N}, K) \neq \emptyset$.*

Theorem 13. Let (\mathcal{N}, K) a weakly reversible poly-PL kinetic system with poly T -matrices T_1, \dots, T_h and $\widehat{\delta} = 0$. Consider an arbitrary poly T -matrix T_k .

(i) if $Z_+(\mathcal{N}, K) \neq \emptyset$ and $x^* \in Z_+(\mathcal{N}, K)$ then

$$Z_+(\mathcal{N}, K) = \left\{ x \in \mathbb{R}_{\geq}^m \mid \log(x) - \log(x^*) \in (\widetilde{S}_j)^\perp \right\}.$$

(ii) if $Z_+(\mathcal{N}, K) \neq \emptyset$ then $|Z_+(\mathcal{N}, K) \cap Q_j| = 1$ for each positive kinetic reactant flux class Q_j .

Corollary. A weakly reversible PY-TIK system is PL-complex balanced.

Proof. Since $(\mathcal{N}, \mathcal{K}_j)$ is a weakly reversible PL-TIK, according to the ZKRD Theorem for PL-TIK [20], it is complex balanced and $Z_+(\mathcal{N}, \mathcal{K}_j) = \left\{ x \in \mathbb{R}_{\geq}^m \mid \log(x) - \log(x^*) \in (\widetilde{S}_j)^\perp \right\}$. The intersection $\cap Z_+(\mathcal{N}, \mathcal{K}_j)$ is, according to Theorem 13 the intersection of $Z_+(\mathcal{N}, K)$ with itself $(h - 1)$ times, and hence equal to $Z_+(\mathcal{N}, K)$. ■

Running Example - Part 3. Considering the weakly reversible kinetic system in the running example, \widehat{T}_1 and \widehat{T}_2 will be

$$\widehat{T}_1 = \begin{bmatrix} 0.5 & 0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \quad \widehat{T}_2 = \begin{bmatrix} -2 & -1 \\ 0 & -1 \\ 1 & 1 \end{bmatrix}$$

Computing the ranks of \widehat{T}_1 and \widehat{T}_2 , we conclude that $(\mathcal{N}, \mathcal{K}_j)$'s are PL-TIK. Thus, by Proposition 11, (\mathcal{N}, K) is PY-TIK. To illustrate Corollary 4.2, note that

$$Z_+(\mathcal{N}, \mathcal{K}_1) = Z_+(\mathcal{N}, \mathcal{K}_2) = \left\{ \left(\frac{\beta^2}{\alpha^2}, y \right) \mid y \in \mathbb{R}_+ \right\} = Z_+(\mathcal{N}, K).$$

Hence, (\mathcal{N}, K) is PL-complex balanced, i.e.,

$$Z_+(\mathcal{N}, K) = Z_{+, PL}(\mathcal{N}, K).$$

4.3 PY-TIK properties as PL complex balanced systems

An important property that can be inferred from the previous Section's results is that PY-TIK systems belong to the set of PY-RDK systems with zero kinetic deficiency:

Proposition 14. *If (\mathcal{N}, K) is a PY-TIK system, then $\tilde{\delta} = 0$.*

Proof. According to the ZKRD Theorem, (\mathcal{N}, K) is unconditionally complex balanced, i.e. $Z_+(\mathcal{N}, K) \neq \emptyset$ for any set of rate constants. According to Proposition 10, for PL complex balanced systems, this is equivalent to zero kinetic deficiency property. ■

Remark. An alternative proof is provided by using the representation of the PY-TIK system with PL-TIK systems, and using their Unconditional Complex Balancing to conclude that their kinetic deficiencies are all 0. The sum formula for kinetic deficiencies then shows the claim.

In the case of power law systems ($h = 1$), weakly reversible PL-RDK systems with zero kinetic deficiency display special properties. For example, Johnston [17] showed that complex balanced equilibria of systems with both network and kinetic deficiencies equal to zero are “translations” of toric steady states of mass action systems. We expect similar special properties in the poly-PL case, too. In the following Sections, properties of PL complex balanced systems regarding linear stability and concentration robustness will be derived, which naturally also hold for PY-TIK systems.

5 Linear stability of complex balanced PY-RDK systems

This section utilizes the STAR-MSD transform of a weakly reversible PY-RDK system in order to expand the results of Boros et al. [3] on linear stability to a subset of $Z_+(\mathcal{N}, K)$ and a subset of PY-RDK system. We first recall some notions of square matrix stability reviewed in [3].

Definition 17. Let S be a linear subspace. A square matrix A with $\text{Im } A \subseteq S$ is said to be **stable on S** if all eigenvalues of the linear map $A|_S : S \rightarrow S$ have negative real part. If all eigenvalues of this linear map have non-positive real part, then the square matrix A is **semistable on S** .

Denote the set of diagonal matrices with positive diagonal by $\mathcal{D}_+ \subseteq \mathbb{R}^{m \times m}$.

Definition 18. Let S be a linear subspace. A square matrix $A \in \mathbb{R}^{m \times m}$ with $\text{Im } A \subseteq S$ is

1. **diagonally stable on S** (respectively, **diagonally semi-stable on S**) if there exists $P \in \mathcal{D}_+$ such that $PA + A^\top P < 0$ on S (respectively, $PA + A^\top P \leq 0$ on S)
2. **D -stable on S** (respectively, **D -semistable on S**) if AD is stable on S (respectively, semistable on S) for all $D \in \mathcal{D}_+$.
3. **diagonally D -stable on S** (respectively, **diagonally D -semistable on S**) if, for all $D \in \mathcal{D}_+$, there exists $P \in \mathcal{D}_+$ such that $PAD + DA^\top P < 0$ on S (respectively, $PAD + DA^\top P \leq 0$ on S).

Recall that for a differentiable species formation rate function f , the **Jacobian matrix** of f at c , denoted by $J(c)$, is the $m \times m$ matrix where $[J(c)]_{ji} = \frac{\partial f_j(c)}{\partial c_i}$.

Definition 19. An equilibrium c^* is **linearly stable** in its stoichiometric class $c^* + S$ if the Jacobian matrix $J(c^*)$ is stable on S . We say that c^* is **diagonally D -stable**, **diagonally stable**, or **D -stable** in $c^* + S$ if $J(c^*)$ is diagonally D -stable, diagonally stable, or D -stable on S , respectively.

One of the main results in [3] was that linear stability of a complex balanced equilibrium of a GMAS system implies uniqueness in a stoichiometric class. The analogous result we have so far is the following:

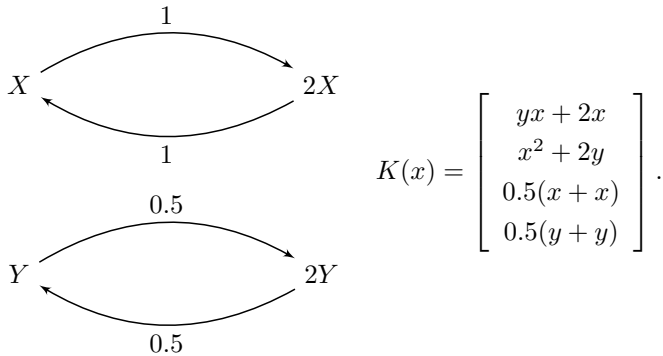
Theorem 15. *Let (\mathcal{N}, K) be a weakly reversible PY-RDK system.*

- (i) *If a PL-complex balanced equilibrium c^* is linearly stable, then it is unique in its stoichiometric class.*

(ii) If (\mathcal{N}, K) is PL-complex balanced, then any linearly stable complex balanced equilibrium is unique in its stoichiometric class.

Proof. To prove (i), note that since c^* is PL-complex balanced, it is a complex balanced equilibrium of (\mathcal{N}^*, K^*) . Since the latter is dynamically equivalent to (\mathcal{N}, K) , c^* is a linearly stable equilibrium for (\mathcal{N}^*, K^*) . According to the GMAS result (i.e. Theorem 10 of [3]), it is unique in its stoichiometric class under \mathcal{N}^* . However, since $S^* = S$, it is also unique in the stoichiometric class of \mathcal{N} . Statement (ii) follows from the equation $Z_{+, \text{PL}}(\mathcal{N}, K) = Z_+(\mathcal{N}, K)$. ■

Example 3. The following is a weakly reversible system with two species X and Y :



The system is PY-RDK. An example of monostationary PL-complex balanced equilibrium is $c^* = (2, 2) \in \cap Z_+(\mathcal{N}, \mathcal{K}_j) = Z_+(\mathcal{N}, K) = \{(x, x) | x \in \mathbb{R}_+\}$. Calculating the Jacobian matrix evaluated at $(2, 2)$, we get

$$\begin{bmatrix}
 -2 & 0 \\
 1 & -1
 \end{bmatrix}.$$

Thus, the eigenvalues are all negative and c^* is linearly stable.

Finally, we briefly state the analogues of Theorems 11 and 13 from [3] for PL-complex balanced PY-RDK systems on cyclic and weakly reversible networks respectively.

Theorem 16. Let (\mathcal{N}, K) be a PL-complex balanced PY-RDK system on

a cyclic network. Let $A = YA_{k=1}\Psi_K$, where Ψ_K is the factor map of K and $A_{k=1}$ is the Laplacian map with all rate constants equal to 1. Then we have the following relationships:

$$\begin{array}{ccc}
 \text{For all rate constants,} & & \text{For all rate constants,} \\
 \text{complex balanced equilibria} & & \text{complex balanced equilibria} \\
 \text{are diagonally stable} & \Rightarrow & \text{are linearly stable} \\
 \text{in their stoichiometric classes.} & & \text{in their stoichiometric classes.} \\
 \Downarrow & & \Downarrow \\
 A \text{ is diagonally } D\text{-stable on } S. & \Rightarrow & A \text{ is } D\text{-stable on } S.
 \end{array}$$

Theorem 17. Let (\mathcal{N}, K) be a PL-complex balanced PY-RDK system on a weakly reversible network. For each cycle C , let $A^C = YA_{k=1}^C\Psi_K$ and S^C be the corresponding stoichiometric subspace. Then we have the following relationships:

$$\begin{array}{ccc}
 \text{For all rate constants,} & & \text{For all rate constants,} \\
 \text{complex balanced equilibria} & & \text{complex balanced equilibria} \\
 \text{are diagonally stable} & \Rightarrow & \text{are linearly stable} \\
 \text{in their stoichiometric classes.} & & \text{in their stoichiometric classes.} \\
 \Downarrow & & \Downarrow \\
 \text{For all cycles } C, & & \text{For all cycles } C, \\
 A^C \text{ is diagonally } D\text{-semistable on } S^C. & \Rightarrow & A^C \text{ is } D\text{-semistable on } S^C.
 \end{array}$$

6 Concentration robustness in PYK systems

In this section, we derive new results about concentration robustness in poly-PL systems after reviewing and consolidating previous ones. We begin with balanced concentration robustness (BCR), where the set of complex balanced equilibria is best understood and a simple computation procedure is available. We then consider sufficient conditions for absolute concentration robustness in PYK systems .

6.1 Concentration robustness in poly-PL systems of CLP type

We recall the general definition of concentration robustness in a species X over a set of positive equilibria Y .

Definition 20. A kinetic system (\mathcal{N}, K) has concentration robustness in a species X over a subset Y of positive equilibria if the concentration value for X is invariant over all equilibria in Y .

Most studied sets have been absolute concentration robustness (ACR) where $Y = E_+(\mathcal{N}, K)$ and balanced concentration robustness (BCR) when $Y = Z_+(\mathcal{N}, K)$.

In the following, we first study balanced concentration robustness in PYK systems of CLP type, i.e. those with $Z_+(\mathcal{N}, K) = \{x \in \mathbb{R}_{>}^{\mathcal{S}} \mid \log x - \log x^* \in P_Z^\perp\}$, with x^* a given complex balanced equilibrium, P_Z the system's flux subspace and P_Z^\perp its parameter subspace. Lao et al derived the following "Species Hyperplane Criterion for BCR":

Theorem 18 (Theorem 3.12, [18]). *Let (\mathcal{N}, K) be a kinetic system, m_{ACR} and m_{BCR} be the number of species with ACR and BCR, respectively. If (\mathcal{N}, K) is a weakly reversible CLP system then it has BCR in a species X if and only if its parameter subspace P_Z^\perp is a subspace of the species hyperplane $\{x \in \mathbb{R}^{\mathcal{S}} \mid x_X = 0\}$. Furthermore, $m_{ACR} \leq m_{BCR} \leq s$.*

The criterion above leads to a simple procedure for determining BCE in a weakly reversible CLP system. If $P_Z^\perp = 0$, then the system has a unique complex balanced equilibrium, which is trivially equivalent to BCR in all species. Otherwise, one constructs a basis of P_Z^\perp , and BCR holds in X if and only if all basis vectors have a zero coordinate in X .

In Proposition 10, we showed that every PL-complex balanced PY-RDK system is a CLP system with $P_Z = \tilde{S}_1 + \cdots + \tilde{S}_h$. Hence, balanced concentration robustness in such PYK systems can be determined by the results reviewed above.

Proposition 6.4 of [18] shows that the same conclusion as in Proposition (10) holds even if the CLP summands are not necessarily PL-RDK. A class of such PLK systems is given by the following result of [11]:

Theorem 19. *Let (\mathcal{N}, K) be a weakly reversible power law kinetic system with a complex balanced PL-RDK decomposition $\mathcal{D} : \mathcal{N} = \mathcal{N}_1 \cup \dots \cup \mathcal{N}_k$ with $P_{Z,i} = \tilde{S}_i$. If \mathcal{D} is incidence independent and the induced covering $\tilde{\mathcal{D}}$ is independent, then (\mathcal{N}, K) is a weakly reversible CLP system with $P_Z = \sum \tilde{S}_i$.*

A PL-NDK system with such PL-RDK decomposition is a subnetwork of Schmitz’s earth pre-industrial carbon cycle model [10]. Such summands can be combined with PL-RDK systems to yield PL-complex balanced PY-NDK systems of CLP type.

If a PL-complex balanced PYK system is absolutely complex balanced, then ACR in a species if and only if BCR in a species. The case of systems with positive non-complex balanced equilibria is discussed in the next section.

6.2 Absolute concentration robustness in poly-PL systems

We first introduce the analogue of PL-complex balanced PYK systems for the study of absolute concentration robustness.

Definition 21. A poly-PL system (\mathcal{N}, K) is **PL-equilibrated (PL-complex balanced)** if $E_+(\mathcal{N}, K) = E_{+,PLE}(\mathcal{N}, K)$ ($Z_+(\mathcal{N}, K) = Z_{+,PLC}(\mathcal{N}, K)$) where

$$E_{+,PLE}(\mathcal{N}, K) = \bigcap_{j \in \overline{1,h}} E_+(\mathcal{N}, K_j) \quad (Z_{+,PLC}(\mathcal{N}, K) = \bigcap_{j \in \overline{1,h}} Z_+(\mathcal{N}, K_j)).$$

Our aim is to derive sufficient conditions for ACR in species of PL-equilibrated systems. These will be based on “low deficiency ACR building blocks” similar to those for PLK systems, which we now briefly recall.

6.2.1 A brief review of ACR in low deficiency PL-RDK systems

The concept of **absolute concentration robustness (ACR)** was first introduced by Shinar and Feinberg in their well-cited paper published in *Science* [24]. ACR pertains to a phenomenon in which a species in a

chemical kinetic system carries the same value for any positive steady state the network may admit regardless of initial conditions. The work of Shinar and Feinberg is influential largely because they established simple yet sufficient criteria for a mass action system to exhibit ACR. In [9], this result is slightly modified to come up with an analogous theorem for PL-RDK systems.

Fortun and Mendoza [8] further investigated ACR in power law kinetic systems and derived novel results that guarantee ACR for some classes of PLK systems. For these PLK systems, the key property for ACR in a species X is the presence of an SF-reaction pair. A pair of reactions in a PLK system is called a **Shinar-Feinberg pair** (or **SF-pair**) in a species X if their kinetic order vectors differ only in X . A subnetwork of the PLK system is of **SF-type** if it contains an SF-pair in X .

An SF-pair is called linked if both reactions lie in a linkage class. It is called non-terminal if both reactant complexes do not lie in terminal strong linkage classes. The following sufficient condition for deficiency zero PL-RDK systems was derived in [9]:

Theorem 20 (Th. 6, [8]). *Let (\mathcal{N}, K) be a deficiency zero PL-RDK with a positive equilibrium. If the system has a linked Sf-pair in a species X , then it has ACR in X .*

We have the following sufficient condition for ACR in larger and higher deficiency PLK systems [18]:

Proposition 21 (Prop. 5.3, [18]). *Let (\mathcal{N}, K) be a power law system with a positive equilibrium and an independent decomposition $\mathcal{N} = \mathcal{N}_1 \cup \dots \cup \mathcal{N}_k$. If there is a subnetwork (\mathcal{N}_i, K_i) of deficiency δ_i with SF-pair in species X such that*

- (i) $\delta_i = 0$ and (\mathcal{N}_i, K_i) is a weakly reversible PL-RDK system with the SF-pair in a linkage class; or
- (ii) $\delta_i = 0$, (\mathcal{N}_i, K_i) is a PL-RDK system, and the SF-pairs's reactant complexes are nonterminal;

then (\mathcal{N}, K) has ACR in X .

Theorem 22 (Shinar-Feinberg Theorem on ACR for PL-RDK systems, [9]). *Let $\mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R})$ be a deficiency-one CRN and suppose that (\mathcal{N}, K) is a PL-RDK system which admits a positive equilibrium. If $y, y' \in \mathcal{C}$ are nonterminal complexes whose kinetic order vectors differ only in species X , then the system has ACR in X .*

6.2.2 Low deficiency ACR building blocks for PYK systems

The key step is the following extension of the SF-pair concept from PLK to PYK:

Definition 22. Let $\{\mathcal{K}_j\}$ the canonical PL-representation of the PYK system (\mathcal{N}, K) and $R_i, R_{i'} \in \mathcal{R}$. The pair of reactions $\{R_i, R_{i'}\}$ is an **SF-pair in the species X** if there is at least one \mathcal{K}_j where the rows differ in X . A PYK system with an SF-pair in X is said to be of **Shinar-Feinberg type** (SF-type) in X .

An SF-pair is called linked if both reactions lie in a linkage class. It is called non-terminal if both reactant complexes do not lie in terminal strong linkage classes.

We derive the deficiency one building block first:

Theorem 23 (SFACR Theorem for PY-RDK_{PLE}). *Let $\{\mathcal{K}_j\}$ be the canonical PL-representation of a deficiency one (\mathcal{N}, K) with $K \in \text{PY-RDK}_{PLE}$. If $E_+(\mathcal{N}, K) \neq \emptyset$ and a non-terminal SF-pair in a species X exists, then the system has ACR in X .*

Proof. We first note that for any kinetic system (\mathcal{N}, K) and a decomposition $\mathcal{N} = \mathcal{N}_1 \cup \dots \cup \mathcal{N}_k$ with $\emptyset \neq E_+(\mathcal{N}, K) = \cap E_+(\mathcal{N}_i, K_i)$, if X has ACR in (\mathcal{N}_i, K_i) , then it has ACR in (\mathcal{N}, K) too. Let (\mathcal{N}^*, K^*) be the STAR-MSC transform of (\mathcal{N}, K) . We have $E_+(\mathcal{N}, \mathcal{K}_j) = E_+(\mathcal{N}_j^*, K^*)$, hence, due to dynamic equivalence, $E_+(\mathcal{N}, K) = E_+(\mathcal{N}^*, K^*)$, and PL-equilibrated implies $E_+(\mathcal{N}^*, K^*) = \cap E_+(\mathcal{N}_j^*, K^*)$. There is at least one j such that a non-terminal SF-pair for (\mathcal{N}_j^*, K^*) exists for the deficiency 1 network \mathcal{N}_j^* which has a positive equilibrium for the PL-RDK kinetics K^* . Hence the subnetwork \mathcal{N}_j^* has ACR in X . It follows that the whole network has ACR in X . ■

An analogous proof can be given for the deficiency zero building block:

Theorem 24 (ACR Theorem for zero deficiency PY-RDK_{PLE}). *Let $\{\mathcal{K}_j\}$ be the canonical PL-representation of a weakly reversible deficiency zero (\mathcal{N}, K) with $K \in \text{PY-RDK}_{\text{PLE}}$. If $E_+(\mathcal{N}, K) \neq \emptyset$ and a non-terminal linked SF-pair in a species X exists, then the system has ACR in X .*

Running Example - Part 4. In the running example, the weakly reversible deficiency zero system has ACR in X . Computing the set of equilibria, we have

$$E_+(\mathcal{N}, K) = \left\{ \left(\frac{\beta^2}{\alpha^2}, y \right) \mid y \in \mathbb{R}_+ \right\}.$$

6.2.3 ACR in larger and higher deficiency PYK systems

We can now provide a sufficient condition for ACR in larger and higher deficiency PYK systems:

Proposition 25. *Let (\mathcal{N}, K) be a poly PL- system with a positive equilibrium and an independent decomposition $\mathcal{N} = \mathcal{N}_1 \cup \dots \cup \mathcal{N}_k$. If there is a subnetwork (\mathcal{N}_i, K_i) of deficiency δ_i with SF-pair in species X such that*

- (i) $\delta_i = 0$ and (\mathcal{N}_i, K_i) is a weakly reversible PY-RDK_{PLE} system with the SF-pair in a linkage class; or
- (ii) $\delta_i = 0$, (\mathcal{N}_i, K_i) is a PY-RDK_{PLE} system, and the SF-pairs' reactant complexes are nonterminal;

then (\mathcal{N}, K) has ACR in X .

Proof. Since the decomposition is independent, it follows from Feinberg's Decomposition Theorem that $E_+(\mathcal{N}, K) = \cap E_+(\mathcal{N}_i, K_i)$. ACR in X in the superset of equilibria $E_+(\mathcal{N}_i, K_i)$ of a building block implies the claim. ■

7 Summary and Outlook

Using tools in chemical reaction network theory (CRNT), this paper assembles relevant results that tackle the dynamical properties of chemical

reaction networks endowed with poly-PL kinetics. Poly-PL kinetic systems consist of nonnegative linear combinations of power law functions. The main approach used in this paper is the construction of power law representations of poly-PL systems in order to apply, expand or mimic existing results in CRNT involving power law kinetic systems. This contribution offers two primary methods in rewriting a poly-PL system into its power law representation: the canonical PL-representation and the STAR-MSK representation. Based from these representations, the following main results are reiterated:

1. For a weakly reversible PY-RDK system, there are rate constants for which the system is complex balanced. In fact, if its canonical PL-representation consists of PL-RDK systems with zero kinetic deficiency, then the system is complex balanced for any set of rate constants. The parametrization of a subset of the set of complex balanced equilibria is provided in Proposition 8. Further, a necessary and sufficient condition for the existence of more than one distinct complex balanced PL-equilibria in a stoichiometric class of a weakly reversible PY-RDK system is established. All these aforementioned results form partial extensions of the GMAS results of Müller and Regensburger [21, 22] to a subset of poly-PL kinetics that are reactant-determined (PY-RDK). Full analogue results for PY-RDK systems with PL-equilibria and PL-complex balanced equilibria sets are collated and presented in Proposition 10.
2. A class of poly-PL systems called PY-TIK systems that are weakly reversible were shown to exhibit PL-complex balancing property. They are precisely the poly-PL systems with zero kinetic reactant deficiency.
3. STAR-MSK transform of a weakly reversible poly-PL kinetic system has led us to the extension of the results of Boros et al. [3] on linear stability to a subset of complex balanced equilibria and a subset of PY-RDK system.
4. The notions of absolute concentration robustness (ACR) and balanced concentration robustness (BCR) are also extended to PL-

equilibrated and PL-complex balanced poly-PL kinetic systems, respectively. The results are expansions of the work of Fortun and Mendoza [8] on deficiency zero ACR, and the detection of ACR and BCR in larger or higher deficiency networks.

As future perspective, one may look at the extension of the multistationarity algorithm for power law kinetic systems [15] to poly-PL systems. The results provided in this paper can be further enlarged to include Hill-type kinetic systems through the transformation introduced in [14].

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A Complex Balancing of RID Kinetic Systems

We derive the Conditional Complex Balancing (CCB) property for any poly-PL kinetics on a weakly reversible network from a general result on RID kinetics.

Definition 23. A rate constant-interaction map decomposable kinetics (RIDK) is a kinetics, such that for each reaction R_j , the coordinate function $K_j : \Omega \rightarrow \mathbb{R}$ can be written in the form $K_j(x) = k_j I_{K,j}(x)$, with $k_j \in \mathbb{R}_{>0}$ (called rate constant) and $\Omega \subset \mathbb{R}^m$. We call the map $I_K : \Omega \rightarrow \mathbb{R}^r$ defined by $I_{K,j}$ as the **interaction map**.

A poly-PL kinetics K is an RIDK, the interaction I_K being the poly-PL function. By definition, an RIDK is called complex factorizable if at each branching point of the network, any branching reaction has the same interaction [23].

We recall three known facts in a lemma:

Lemma 1. Consider the chemical kinetic system (\mathcal{N}, K) .

- (i) A network \mathcal{N} is weakly reversible if and only if $\text{Ker } I_a$ contains a positive vector.
- (ii) A weakly reversible network \mathcal{N} is positive dependent.
- (iii) For any RIDK on a positively dependent network \mathcal{N} , there are rate constants so that (\mathcal{N}, K) has a positive equilibrium.

The proofs of (i) and (ii) can be found in [4] and [7], respectively. The proof in [7] is readily adapted to show (iii).

Theorem 26 (CCB for RIDK on weakly reversible networks). Let K be an RID kinetics on a weakly reversible network \mathcal{N} . Then there exist rate constants such that (\mathcal{N}, K) is complex balanced, i.e. $Z_+(\mathcal{N}, K) \neq \emptyset$.

Proof. Since a weakly reversible network is positive dependent, according to Lemma 1 (ii) and (iii), there are rate constants k'_q such that (\mathcal{N}, K) has a positive equilibrium x^* . Let I_K be the interaction function of K . Furthermore, according to Lemma 1 (i), weak reversibility implies that there is a positive vector $b \in \text{Ker } I_a$. Let $C = \text{diag}(b_1/I_{K,1}(x^*), \dots, b_r/I_{K,r}(x^*))$ and $k'_q = (Ck^*)_q$. Then $I_{a,q}(k'_q I_{K,q}(x^*)) = I_{a,q}(b_q/I_{K,q}(x^*))k'_q I_{K,q}(x^*) = k'_q I_a(b) = 0$. Hence, for rate constants k'_q , x^* is a complex balanced equilibrium, and the claim is established. \blacksquare

B Nomenclature

We list some of the symbols and acronyms used in the paper.

List of Symbols

δ	Deficiency
K	Kinetics of a CRN
Ψ_K	Factor map of a kinetics
$\text{sum} \langle \mathbf{B}_j \rangle$	Image span sums
I_a	Incidence map/matrix
J	Jacobian matrix
$\tilde{\delta}$	Kinetic deficiency
F	Kinetic order matrix
A_k	k -Laplacian matrix
Y	Map of complexes
$Z_+(\mathcal{N}, K)$	Set of complex balanced equilibria
$E_{+,PL}(\mathcal{N}, K)$	Set of PL-complex balanced equilibria
$E_{+,PL}(\mathcal{N}, K)$	Set of PL-equilibria
$E_+(\mathcal{N}, K)$	Set of positive equilibria
N	Stoichiometric matrix

Abbreviations

ACR	Absolute concentration robustness
BCR	Balanced concentration robustness
CKS	Chemical kinetic system
CRN	Chemical reaction network
CF	Complex factorizable
CCB	Conditional complex balancing
GMAS	Generalized mass action system
MAK	Mass action kinetic
NF	Non-complex factorizable
NDK	Non-reactant determined kinetics
PLC	PL-complex balanced
PLE	PL-equilibrated
PY	Poly-PL
PYK	Poly-PL kinetic system
PL	Power law
RID	Rate constant-interaction map decomposable
RDK	Reactant-determined kinetics
SF	Shinar-Feinberg
STAR-MSC	S -invariant termwise addition of reactions via maximal stoichiometric coefficients
UCB	Unconditional complex balancing