Robustness in Power-law Kinetic Systems with Reactant-determined Interactions

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Abstract. Robustness against the presence of environmental disruptions can be observed in many systems of chemical reaction network. However, identifying the underlying components of a system that give rise to robustness is often elusive. The influential work of Shinar and Feinberg established simple yet subtle network-based conditions for absolute concentration robustness (ACR), a phenomena in which a species in a mass-action system has the same concentration for any steady state the network may admit. In this contribution, we extend this result to embrace kinetic systems more general than mass-action systems, namely, power-law kinetic systems with reactant-determined interactions (denoted by “PL-RDK”). In PL-RDK, the kinetic order vectors (which we call “interactions”) of reactions with the same reactant complex are identical. As illustration, we considered a scenario in the pre-industrial state of global carbon cycle. A power-law approximation of the dynamical system of this scenario is found to be dynamically equivalent to an ACR-possessing PL-RDK system.

Keywords: Absolute concentration robustness · Chemical reaction network · Power-law kinetics · Reactant-determined interactions · Carbon cycle model.

1 Introduction

Robustness may be generally defined as a system-level dynamical property that allows a system to sustain its functions despite changes in internal and external conditions. This feature, in fact, is fundamental and ubiquitous in biological processes, including cellular networks and entire organisms.
Sustaining the functionality of a system amidst disruptions often depends on its components [8], yet interestingly, robustness is a phenomena that cannot be understood by looking at the individual components [12].

In a well-cited paper published in *Science*, Shinar and Feinberg [16] presented sufficient structure-based conditions for a chemical reaction network (CRN) to display absolute concentration robustness (ACR) on a particular species. If the evolution of a CRN is modelled with ordinary differential equations with mass-action kinetics (MAK), the CRN is said to exhibit ACR for a species if the concentration of that species is the same for any positive steady state the system may admit.

Shinar and Feinberg related the capacity of a CRN to exhibit ACR to a structural index called the deficiency. This non-negative parameter has been the center of many powerful results in Chemical Reaction Network Theory, a theoretical body of work that associates the structure of a CRN to the dynamical behaviour of the system [9,10]. CRNT employs mathematical methods from graph theory, linear algebra, group theory and the theory of ordinary differential equations. In CRNT, chemical reaction networks are viewed as digraphs whose vertices (called complexes) are mapped to non-negative vectors representing compositions of chemical species and whose arcs represent chemical reactions between them. The Shinar-Feinberg Theorem on ACR is stated as follows:

\[
\text{Consider a mass-action system that admits a positive steady state and suppose that the deficiency of the underlying reaction network is one. If there are two nonterminal nodes in the network that differ only in species S, then the system has absolute concentration robustness in S.}
\]

Despite the prevalence of MAK in many systems of reaction network, it is still limited since it only holds for elementary reactions in homogeneous and isothermal solutions. Systems such as intracellular environment, for instance, are characterized by molecular crowding for which power-law kinetics (PLK) is preferred than MAK [13]. Savageau [15] and Voit [18,19] highlighted the advantages of using power-law formalism for modelling biochemical systems. In this light, many CRN-based results on PLK systems are established ([6,11,13,17] among others), some of which are extensions or modifications of existing results on MAK systems.

Here, we show that the Shinar-Feinberg Theorem on ACR extends to a class of PLK systems, namely power-law kinetic systems with reactant-determined interactions (denoted by “PL-RDK”). PL-RDK systems are kinetic systems with power-law rate functions whose kinetic order vectors are identical for branching reactions (that is, reactions with the same reactant complex). Since the kinetic orders of the mass-action rate functions are precisely the stoichiometric coefficients of the reactant complex, one can see that MAK is a special case of PL-RDK.

As application, we employ the theorem to a power-law approximation of the ODE system corresponding to a specific scenario in the pre-industrial carbon cycle model developed by Anderies et al. [1]. Specifically, in the pre-industrial
scenario where there are anthropogenic causes that reduce the capacity of terrestrial carbon pool to store carbon, the power-law approximation leads to an ACR possessing PL-RDK system.

The rest of the paper is organized as follows: Section 2 assembles preliminary concepts in Chemical Reaction Network Theory required in stating and proving the results. Section 3 discusses the extension of the Shinar-Feinberg Theorem on ACR for PL-RDK systems. Section 4 applies the main result obtained from the previous section to a carbon cycle model. In Section 5, we summarize our results and outline some research perspectives.

2 Fundamentals of Chemical Reaction Networks and Kinetic Systems

We recall some fundamental notions about chemical reaction networks (CRNs) and chemical kinetic systems (CKS) assembled in [5,17]. Some concepts introduced by Feinberg in [9,10] are also reviewed.

**Notation.** We denote the real numbers by $\mathbb{R}$, the non-negative real numbers by $\mathbb{R}_{\geq 0}$ and the positive real numbers by $\mathbb{R}_{> 0}$. Objects in the reaction systems are viewed as members of vector spaces. Suppose $\mathcal{I}$ is a finite index set. By $\mathbb{R}^\mathcal{I}$, we mean the usual vector space of real-valued functions indexed by $\mathcal{I}$. For $x \in \mathbb{R}^\mathcal{I}$, the $i$th coordinate of $x$ is denoted by $x_i$, where $i \in \mathcal{I}$. The sets $\mathbb{R}_{\geq 0}^\mathcal{I}$ and $\mathbb{R}_{> 0}^\mathcal{I}$ are called the non-negative and positive orthants of $\mathbb{R}^\mathcal{I}$, respectively. Addition, subtraction, and scalar multiplication in $\mathbb{R}^\mathcal{I}$ are defined in the usual way. If $x, y \in \mathbb{R}_{> 0}^\mathcal{I}$, we define $x^y \in \mathbb{R}_{> 0}^\mathcal{I}$ by $x^y = \prod_{i \in \mathcal{I}} x_i^{y_i}$. The vector $\log x \in \mathbb{R}^\mathcal{I}$, where $x \in \mathbb{R}_{> 0}^\mathcal{I}$, is given by $(\log x)_i = \log x_i$, for all $i \in \mathcal{I}$. If $x, y \in \mathbb{R}^\mathcal{I}$, the standard scalar product $x \cdot y \in \mathbb{R}$ is defined by $x \cdot y = \sum_{i \in \mathcal{I}} x_i y_i$. By the support of $x \in \mathbb{R}^\mathcal{I}$, denoted by $\text{supp } x$, we mean the subset of $\mathcal{I}$ assigned with non-zero values by $x$. That is, $\text{supp } x := \{ i \in \mathcal{I} | x_i \neq 0 \}$.

We formally define CRN as a digraph with vertex-labelling (its stoichiometry).

**Definition 1.** A chemical reaction network is a digraph $(\mathcal{C}, \mathcal{R})$ where each vertex has positive degree and stoichiometry, i.e. there is a finite set $\mathcal{I}$ (whose elements are called species) such that $\mathcal{C}$ is a subset of $\mathbb{R}_{\geq 0}^\mathcal{I}$. Each vertex is called a complex and its coordinates in $\mathbb{R}_{\geq 0}^\mathcal{I}$ are called stoichiometric coefficients. The arcs are called reactions. We denote the number of species with $m$, the number of complexes with $n$ and the number of reactions with $r$.

This definition of a CRN is equivalent to the usual definition as a triple $\mathcal{N} = (\mathcal{I}, \mathcal{C}, \mathcal{R})$ in [9] with the requirement $\mathcal{I} = \bigcup \text{supp } y$ for $y \in \mathcal{C}$, i.e., each species appears in at least one complex.

In the reaction $y \rightarrow y'$, 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 with \( \ell \), 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.

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 \( \mathbb{R}^S \) defined by

\[
S := \text{span} \{ y' - y \in \mathbb{R}^S \mid y \rightarrow y' \in \mathcal{R} \}.
\]

The rank of the CRN, \( s \), is defined as \( s = \dim S \).

Many features of CRNs can be examined by working in terms of finite dimensional spaces \( \mathbb{R}^S \) (species space), \( \mathbb{R}^C \) (complex space), and \( \mathbb{R}^R \) (reaction space). Suppose the set \( \{ \omega_i \in \mathbb{R}^I \mid i \in I \} \) forms the standard basis for \( \mathbb{R}^I \) where \( I = S, C \) or \( R \). We now recall four maps relevant in the study of CRNs: map of complexes, incidence map, stoichiometric map and Laplacian map.

**Definition 2.** Let \( \mathcal{N} = (S, C, R) \) be a CRN. The map of complexes \( Y : \mathbb{R}^C \rightarrow \mathbb{R}^S \) maps the basis vector \( \omega_y \) to the complex \( y \in C \). The incidence map \( I_a : \mathbb{R}^R \rightarrow \mathbb{R}^C \) is the linear map defined by mapping for each reaction \( r : y \rightarrow y' \in \mathcal{R} \), the basis vector \( \omega_r \) to the vector \( \omega_y' - \omega_y \in C \). The stoichiometric map \( N : \mathbb{R}^R \rightarrow \mathbb{R}^S \) is defined as \( N = Y \circ I_a \). The linear transformation \( A_k : \mathbb{R}^C \rightarrow \mathbb{R}^C \) called Laplacian map is the mapping defined by

\[
A_k x := \sum_{y \rightarrow y' \in \mathcal{R}} k_{y \rightarrow y'} x_y (\omega_{y'} - \omega_y),
\]

where \( x_y \) refers to the \( y \)-th component of \( x \in \mathbb{R}^C \) relative to the standard basis.

The following result, named as the STLK by Arceo et al. in [5], is crucial in deriving important results in CRNT [9,10].

**Proposition 1 (Structure Theorem of the Laplacian Kernel (STLK), Prop. 4.1 [9]).** Let \( \mathcal{N} = (S, C, R) \) be a CRN with terminal strong linkage classes \( C^1, C^2, ..., C^t \). Let \( k \in \mathbb{R}^R_{>0} \) and \( A_k \) its associated Laplacian. Then \( \ker A_k \) has a basis \( b^1, b^2, ..., b^t \) such that \( \text{supp } y^i = C^i \) for all \( i = 1, 2, ..., t \).

A non-negative integer, called the deficiency, can be associated to each CRN. The deficiency of a CRN, denoted by \( \delta \), is the integer defined by \( \delta = n - \ell - s \). This index has been the center of many studies in CRNT due to its relevance in the dynamic behaviour of the system. In [9], Feinberg provided a geometric interpretation of deficiency: \( \delta = \dim(\ker Y \cap \text{Im } I_a) \). From this fact and the STLK, the following result follows.

**Corollary 1.** Let \( \mathcal{N} = (S, C, R) \) be a CRN with deficiency \( \delta \) and \( t \) terminal strong linkage classes. Then for each \( k \in \mathbb{R}^R_{>0} \),

\[
\dim(\ker YA_k) \leq \delta + t.
\]
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.

**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 $j \in \mathcal{R}$, where $\Omega_K$ is a set such that $\mathbb{R}_{>0} \subseteq \Omega_K \subseteq \mathbb{R}_{\geq 0}$, and $c \land d \in \Omega_K$ whenever $c, d \in \Omega_K$, and

$$K_j(c) \geq 0, \quad \text{for all } c \in \Omega_K.$$ 

A kinetics for a network $\mathcal{N}$ is denoted by $K = [K_1, K_2, \ldots, K_r]^\top : \Omega_K \rightarrow \mathbb{R}_{\geq 0}^r$. The pair $(\mathcal{N}, K)$ is called the chemical kinetic system (CKS).

The above definition is adopted from [20]. It is expressed in a more general context than what one typically finds in CRNT literature. For power-law kinetic systems, one sets $\Omega_K = \mathbb{R}_{>0}$. Here, we focus on the kind of kinetics relevant to our context:

**Definition 4.** A chemical kinetics is a kinetics $K$ satisfying the positivity condition:

For each reaction $j : y \rightarrow y' \in \mathcal{R}$, $K_j(c) > 0$ if and only if $\text{supp } y \subset \text{supp } c$.

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

**Definition 5.** The species formation rate function (SFRF) of a chemical kinetic system (CKS) is the vector field

$$f(c) = NK(c) = \sum_{y \rightarrow y'} K_{y \rightarrow y'}(c)(y' - y).$$

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 $\mathbb{R}_{>0}$ for which $f(c^*) = 0$. The set of positive equilibria of a chemical kinetic system is denoted by $E_+(\mathcal{N}, K)$.

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

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

$$K_i(x) = k_i x^{F_i}, \quad \forall i = 1, \ldots, r$$

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 $i, j$ with identical reactant complexes, the corresponding rows of kinetic orders in $F$ are identical, i.e., $F_{ik} = F_{jk}$ for $k = 1, \ldots, m$. 
An example of PL-RDK is the well-known mass-action kinetics (MAK), where the kinetic order matrix is the transpose of the matrix representation of the map of complexes $Y$. That is, a kinetics is a MAK if

$$K_i(c) = k_i x^{Y_{i,j}} \text{ for all } i \to j \in \mathcal{R}$$

where $k_i \in \mathbb{R}_{>0}$, called rate constants. Note that $Y_{i,j}$ pertains to the stoichiometric coefficients of a reactant complex $i \in \mathcal{C}$.

**Remark 1.** In [5], Arceo et al. discussed several sets of kinetics of a network and drew a “kinetic landscape”. They identified two main sets: the complex factorizable (CF) kinetics and its complement, the non-complex factorizable (NF) kinetics. CF kinetics generalize the key structural property of MAK – that is, the species formation rate function decomposes as

$$\frac{dx}{dt} = Y \circ A_k \circ \Psi_k,$$

where $Y$ is the map of complexes, $A_k$ is the Laplacian map, and $\Psi_k : \mathbb{R}^\mathcal{S} \to \mathbb{R}^\mathcal{C}$ is the analogue of MAK’s monomial map. In the set of power-law kinetics, PL-RDK is the subset of CF kinetics.

We recall the definition of the $m \times n$ matrix $\tilde{Y}$ from the work of Müller and Regensburger [13,14]: For a reactant complex, the column of $\tilde{Y}$ is the transpose of the kinetic order matrix row of the complex’s reaction, otherwise (i.e., for non-reactant complexes), the column is 0. We form the $T$-matrix of a PL-RDK system by truncating away the columns of the non-reactant complexes in $\tilde{Y}$, obtaining an $m \times n_r$ matrix, where $n_r$ denotes the number of reactant complexes [17].

### 3 Absolute Concentration Robustness in PL-RDK Systems

To illustrate absolute concentration robustness, we consider the following toy model:

![Toy model diagram](image)

(1)

The map depicts a biochemical system involving transfer of material from two pools: $X_2$ to $X_1$ and $X_1$ to $X_2$, but with $X_2$ regulating the second process. Suppose the system evolves according to the following set of ODEs:

$$\begin{align*}
x_1' &= k_1 x_2^{0.8} - k_2 x_1^{0.5} x_2^{0.8} \\
x_2' &= -k_1 x_2^{0.8} + k_2 x_1^{0.5} x_2^{0.8}
\end{align*}$$

(2)
The positive equilibrium of the system is attained when

\[ X_1 = \left( \frac{k_1}{k_2} \right)^2, \]
\[ X_2 = \Gamma - \left( \frac{k_1}{k_2} \right)^2, \]

where \( \Gamma \) is the conserved total concentration. Equation (3) indicates that whenever \( \Gamma > \left( \frac{k_1}{k_2} \right)^2 \), a positive steady state exists. Furthermore, since \( X_1 \) has the same value in any steady state, the system exhibits ACR in \( X_1 \).

We define absolute concentration robustness (ACR) in PL-RDK systems as follows:

**Definition 7.** A PL-RDK system \( (\mathcal{N}, K) \) has absolute concentration robustness (ACR) in species \( X \in \mathcal{S} \) if there exists \( c^* \in E_+(\mathcal{N}, K) \) and for every other \( c^{**} \in E_+(\mathcal{N}, K) \), we have \( c^{**}_X = c^*_X \).

The following proposition adapts Theorem S3.15 found in supplementary online material of the paper of Shinar and Feinberg [16] to deal with PL-RDK systems.

**Proposition 2.** Let \( \mathcal{N} = (\mathcal{S}, \mathcal{C}, \mathcal{R}) \) be a deficiency-one CRN. Suppose that \( (\mathcal{N}, K) \) is a PL-RDK system which admits a positive equilibrium \( c^* \). If \( y, y' \in \mathcal{C} \) are nonterminal complexes, then each positive equilibrium \( c^{**} \) of the system satisfies the equation

\[ (T_{y} - T_{y'}) \cdot \log \left( \frac{c^{**}}{c^*} \right) = 0. \]  

We largely reproduce the proof of Shinar and Feinberg in the said supplementary material of their paper. Since in their proof, the sums are often taken over all complexes, we use the notation of Müller and Regensburger in [1314]:

\[ \bar{Y} = \left[ \begin{array}{c} T \mid 0 \end{array} \right], \]

adjoining \( n - n_r \) zero columns for the non-reactant complexes, where \( n_r \) denotes the number of reactant complexes. Furthermore, we write \( \bar{y} \) for \( \bar{Y}_{y} \).

**Proof.** Assume that \( c^* \) is a positive steady state of the PL-RDK system \( (\mathcal{N}, K) \). That is,

\[ \sum_{y \rightarrow y' \in \mathcal{R}} k_{y \rightarrow y'}(c^*)\bar{y}(y' - y) = 0. \]  

For each \( y \rightarrow y' \in \mathcal{R} \), define the positive number \( \kappa_{y \rightarrow y'} \) by

\[ \kappa_{y \rightarrow y'} := k_{y \rightarrow y'}(c^*)\bar{y}(y' - y). \]  

Thus, we obtain

\[ \sum_{y \rightarrow y' \in \mathcal{R}} \kappa_{y \rightarrow y'}(y' - y) = 0. \]
Suppose that $c^{**}$ is also a positive equilibrium of the system. Hence,

$$\sum_{y \rightarrow y' \in \mathcal{R}} k_{y \rightarrow y'}(c^{**}) \tilde{\omega}(y' - y) = 0.$$  \hspace{1cm} (8)

Define

$$\mu := \log c^{**} - \log c^*.$$  \hspace{1cm} (9)

With $\kappa \in \mathbb{R}_{>0}$ given by Equation (6) and $\mu$ given by Equation (9), it follows from Equation (8) that

$$\sum_{y \rightarrow y' \in \mathcal{R}} \kappa_{y \rightarrow y'} e^{\tilde{\omega} \mu} (y' - y) = 0.$$  \hspace{1cm} (10)

Let $1^\mathcal{E} \in \mathbb{R}^\mathcal{E}$ such that

$$1^\mathcal{E} = \sum_{y \in \mathcal{E}} \omega_y.$$  \hspace{1cm}

Observe that Equations (7) and (10) can be respectively written as

$$Y A_\kappa 1^\mathcal{E} = 0, \text{ and } Y A_\kappa \left( \sum_{y \in \mathcal{E}} e^{\tilde{\omega} \mu} \omega_y \right) = 0.$$  \hspace{1cm}

Equivalently,

$$1^\mathcal{E} \in \text{Ker} Y A_\kappa, \text{ and } \sum_{y \in \mathcal{E}} e^{\tilde{\omega} \mu} \omega_y \in \text{Ker} Y A_\kappa.$$  \hspace{1cm} (11, 12)

Therefore, $c^*$ and $c^{**}$ are positive equilibria of the PL-RDK system $(\mathcal{N}, K)$ if and only if Equations (11) and (12) hold. From Corollary 1, we have

$$\dim(\text{Ker} Y A_\kappa) \leq 1 + t.$$  \hspace{1cm} (13)

for the CRN under consideration. Let $\{b^1, b^2, \ldots, b^t\} \subset \mathbb{R}_{\geq 0}^\mathcal{E}$ be a basis for $\text{Ker} A_\kappa$ as in Proposition 1 (STLK). Since $\text{Ker} A_\kappa \subseteq \text{Ker} Y A_\kappa$, this basis of $\text{Ker} A_\kappa$ can be extended to form a basis of $\text{Ker} Y A_\kappa$. Recall from Equation (11) that $1^\mathcal{E}$ is in $\text{Ker} Y A_\kappa$. We assert that the set $\{1^\mathcal{E}, b^1, b^2, \ldots, b^t\}$ is a basis for $\text{Ker} Y A_\kappa$ (and hence, equality holds in Equation (13)). This follows if

$$1^\mathcal{E} \notin \text{Span} \{b^1, b^2, \ldots, b^t\}.$$  \hspace{1cm} (14)

From Proposition 1, every element of $\text{Ker} A_\kappa$ must have its support contained entirely in the set of terminal complexes. However, the support of $1^\mathcal{E}$ consists of all complexes. By assumption, there are nonterminal complexes and hence, $1^\mathcal{E}$ cannot lie in $\text{Ker} A_\kappa$ (i.e., Equation (14) holds).
From Equation (12), there exist scalars $\lambda_0, \lambda_1, \ldots, \lambda_t$ such that

$$
\sum_{y \in \mathcal{C}} e^{\tilde{y} \cdot \mu} y = \lambda_0 \mathbf{1}^{\mathcal{C}} + \sum_{i=1}^{t} \lambda_i b^i. \tag{15}
$$

Observe that each vector $b^i, i = 0, 1, \ldots, t$, has its support entirely on terminal complexes. This fact, along with Equation (15), implies that for each pair of nonterminal complexes $y \in \mathcal{C}$ and $y' \in \mathcal{C}$, we have

$$
\tilde{y} \cdot \mu = \tilde{y}' \cdot \mu. \tag{16}
$$

Since $y$ and $y'$ are nonterminal, they are reactant complexes. Hence, Equation (16) may be written as

$$
T_{-,y} \cdot \mu = T_{-,y'} \cdot \mu, \tag{17}
$$

which is equivalent to Equation (4) in Theorem 2.

The extension of the Shinar-Feinberg Theorem on ACR to PL-RDK systems is stated as follows.

**Theorem 1.** Let $\mathcal{N} = (\mathcal{X}, \mathcal{C}, \mathcal{R})$ 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 interactions differ only in species $X$, then the system has ACR in $X$.

By *interactions*, we refer to the associated kinetic order vectors of the complexes.

**Proof.** Suppose $c^*$ and $c^{**}$ are positive equilibria of the PL-RDK system $(\mathcal{N}, K)$. Observe that since $y, y' \in \mathcal{C}$ are nonterminal complexes whose interactions differ only in species $X$, we have

$$
T_{-,y} - T_{-,y'} = kX
$$

for some positive integer $k$. Thus Equation (4) reduces to

$$
k(\log c^*_X - \log c^{**}_X) = 0.
$$

It follows that

$$
c^*_X = c^{**}_X.
$$

That is, the system has ACR in species $X$.

The ODE system in Equation (2) can be translated into a dynamically equivalent CRN with associated kinetic order matrix by employing the notion of **total CRN representation of Generalized Mass Action (GMA) systems**, proposed by Arceo et al. [5]. GMA system is a canonical framework used in Biochemical Systems Theory (BST) wherein every mass transfer rate is approximated separately with a power-law term, and these terms are added together, with a plus sign for incoming fluxes and a minus sign for outgoing fluxes [18,19].
For BST-related concepts, the reader may refer to the BST tutorial in the Appendix of Arceo et al. [3].

The total CRN representation of a GMA system allows for the CRN-based analysis of the dynamical system. Viewed as a GMA system, the set of ODEs in (2) has the following total CRN representation:

\[
\begin{align*}
R_1 &: X_2 \xrightarrow{k_1} X_1 \\
R_2 &: X_1 + X_2 \xrightarrow{k_2} 2X_2
\end{align*}
\]  

with associated kinetic order matrix \( F \) given by

\[
F = R_1 \begin{bmatrix} x_1 & x_2 \\ 0 & 0.8 \end{bmatrix} R_2 \begin{bmatrix} 0.5 & 0.8 \end{bmatrix}.
\]

The CRN in (18) is a deficiency-one network with nonterminal complexes \( X_1 + X_2 \) and \( X_2 \) whose interactions (or kinetic order vectors) differ only in \( X_1 \). The previous theorem indicates ACR in \( X_1 \), which agrees with the computation in (3).

The following simple proposition provides some examples for the ACR theorem for PL-RDK systems. As preparation, we recall some notions from [4,17] which are used in the result. A power-law kinetics is said to be reactant set linear independent (of type PL-RLK) if the columns of \( T \) are linearly independent. We also recall the reactant matrix \( Y_{res} \), which is obtained from the matrix representation of \( Y \) by removing the columns corresponding to non-reactant complexes. Its image \( \text{Im} \ Y_{res} \) is called the reactant subspace \( R \), whose dimension \( q \) is called the reactant rank of the CRN. The reactant deficiency \( \delta_r \) is the difference between the number of reactant complexes \( n_r \) and the reactant rank \( q \).

**Proposition 3.** Let \((\mathcal{P}, \mathcal{C}, \mathcal{R})\) be a deficiency-one reaction network, which with PL-RDK admits a positive equilibrium. Suppose the network has zero reactant deficiency, two nonterminal complexes \( y, y' \in \mathcal{C} \) differing only in \( X \) and the map

\[
\bar{y} := TY_{res}^{-1} : R \rightarrow \text{Im} \ T
\]

is given by

\[
\bar{y}(x_1, x_2, \ldots, x_m) = (a_1x_1, a_2x_2, \ldots, a_mx_m), \quad a_i \neq 0.
\]

Then the system is PL-RLK and has ACR in \( X \).

**Proof.** Since \( \bar{y} \) is an isomorphism, \( T = \bar{y}Y_{res} \) is also an isomorphism. This implies that the system is PL-RLK. The interaction difference is \((0, \ldots, ka_X, \ldots, 0)\) so that the ACR Theorem’s condition is fulfilled.
4 Application to a Carbon Cycle Model

The pre-industrial carbon cycle model of Anderies et al. [1] is a simple mass balance which involves three interacting carbon pools: land, atmosphere and ocean. In our previous work [11], we reviewed the model’s design and underlying assumptions and described the parameters and ODEs present in the pre-industrial state of the carbon cycle model. We also approximated all rate processes by products of power-law functions in order to obtain a GMA system approximation of the original system. The resulting ODEs of the approximation is given in (19):

\[
\begin{align*}
\dot{A}_1 &= k_1 A_1^{p_1} A_2^{q_1} - k_2 A_1^{p_2} A_2^{q_2} \\
\dot{A}_2 &= k_2 A_1^{p_2} A_2^{q_2} - k_1 A_1^{p_1} A_2^{q_1} - a_m A_2 + a_m \beta A_3 \\
\dot{A}_3 &= a_m A_2 - a_m \beta A_3,
\end{align*}
\]

(19)

Pictorially, the GMA system can be depicted using a biochemical map. The map consists of nodes that represent carbon pools, solid arrows that indicate transfer of carbon, and dashed arrows that indicate if a pool affects or modulates a process. Figure 1 presents the biochemical map of the model of interest.

![Biochemical map of the pre-industrial carbon cycle model of Anderies et al.](image)

Fig. 1. Biochemical map of the pre-industrial carbon cycle model of Anderies et al. [1]

In [11], we also obtained (using total CRN representation of [5]) the following deficiency-one CRN representation for the model:

\[
\begin{align*}
A_1 + 2A_2 &\rightarrow 2A_1 + A_2 \\
A_1 + A_2 &\rightarrow 2A_2 \\
A_2 &\rightleftharpoons A_3
\end{align*}
\]

(20)

Its associated kinetic order matrix is the transpose of the following \(T\)-matrix:

\[
T = \begin{bmatrix}
p_1 & p_2 & 0 & 0 & \text{\(A_1\)} \\
q_1 & q_2 & 1 & 0 & \text{\(A_2\)} \\
0 & 0 & 0 & 1 & \text{\(A_3\)}
\end{bmatrix}
\]

(21)

In the Appendix, it is shown that there is a scenario in the pre-industrial state leading to a GMA system approximation such that the interaction of the nonterminal vertices \(A_1 + 2A_2\) and \(A_1 + A_2\) differ only in \(A_2\); that is, \(p_1 - p_2 = 0\) and \(q_1 - q_2 \neq 0\). In particular, this occurs when the human terrestrial carbon
off-take term (which accounts for human activities that reduce the capacity of terrestrial pool to capture carbon such as deforestation and land-use change) vanishes. Assuming the existence of a steady state, the Shinar-Feinberg Theorem for PL-RDK indicates that the system has ACR in $A_2$. In fact, when $p_1 = p_2$, steady state computation of the system in \[19\] yields the following equilibria set for the system:

$$E_+(\mathcal{N}, K) = \left\{ \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} \in \mathbb{R}_{>0}^3 \mid \begin{align*}
A_2 &= \left(\frac{k_2}{k_1}\right)^{\frac{1}{q_1-q_2}}, \\
A_3 &= \frac{1}{\beta} \left(\frac{k_2}{k_1}\right)^{\frac{1}{q_1-q_2}}, \\
A_1 &= A_0 - \left(1 + \frac{1}{\beta}\right) \left(\frac{k_2}{k_1}\right)^{\frac{1}{q_1-q_2}}
\end{align*} \right\},$$

where $A_0$ = total (conserved) carbon at pre-industrial state.

5 Conclusion and Outlook

In conclusion, we summarize our results and outline some perspectives for further research.

1. We modified the Shinar-Feinberg Theorem on mass-action system to embrace PL-RDK systems, a kinetic system more general than mass-action systems.
2. The theorem is applied to a power-law approximation of Anderies et al.’s Earth’s carbon cycle in its pre-industrial state. Accordingly, there is a scenario in the pre-industrial state that yields a power-law approximation where there is ACR in the atmospheric carbon pool. Specifically, when the human offtake coefficient, which accounts for the which accounts for human activities that reduce the capacity of terrestrial pool to sequester carbon, vanishes, the power-law approximation leads to an ACR-possessing PL-RDK system.
3. The investigation of other forms of “concentration robustness” identified by Dexter et al. [7] for PL-RDK systems offers a further interesting research perspective.
4. The extension of the stochastic analysis of CRNs with ACR of Anderson et al. [2] for PL-RDK systems is another promising area for further investigation.

Acknowledgements

NTF acknowledges the support of the Department of Science and Technology-Science Education Institute (DOST-SEI), Philippines through the ASTHRDP Scholarship grant and Career Incentive Program (CIP). ARL and LFR held research fellowships from De La Salle University and would like to acknowledge the support of De La Salle University’s Research Coordination Office.
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A Pre-industrial Carbon Cycle Model of Anderies et al.

The complete set of ODEs for the pre-industrial state is given by

\[
\begin{align*}
\dot{A}_1 &= r_{tc}[P(t) - R(t)]A_1 \left[1 - \frac{A_1}{k}\right] - \alpha A_1 \\
\dot{A}_2 &= r_{tc}[R(t) - P(t)]A_1 \left[1 - \frac{A_1}{k}\right] + \alpha A_1 - a_m A_2 + a_m \beta A_3 \\
\dot{A}_3 &= a_m A_2 - a_m \beta A_3.
\end{align*}
\]

(22)

where

\[
\begin{align*}
P(t) &= a_f A_2(t)^{b_f} \cdot \left[a_p \cdot (a_T A_2(t) + b_T)^{b_p} \cdot e^{-c_p \cdot (a_T A_2(t) + b_T)}\right] \\
R(t) &= \left[a_r \cdot (a_T A_2(t) + b_T)^{b_r} \cdot e^{-c_r \cdot (a_T A_2(t) + b_T)}\right].
\end{align*}
\]

For the description of the parameters, the reader is referred to [1] and the Appendix of [11]. The parameter values are identical to the values used in [11] but with $\alpha = 0$. This particular parameter is assigned as the human terrestrial carbon off-take rate. It is associated to human activities such as clearing, burning or farming, which reduce the capacity of land to capture carbon.

A power-law approximation of the ODE system at an operating point is obtained to generate a Generalized Mass Action (GMA) System [18,19]. Mathematically, GMA system approximation is equivalent to Taylor approximation up to the linear term in logarithmic space. The function $V(X_1, X_2, \ldots, X_m)$ can be approximated by

\[
V(X_1, X_2, \ldots, X_m) \approx \alpha X_1^{p_1} X_2^{p_2} \cdots X_m^{p_m}
\]

at an operating point where

\[
p_i = \frac{\partial V}{\partial X_i} \cdot \frac{X_i}{V} \quad \text{and} \quad \alpha = V(X_1, X_2, \ldots, X_m)X_1^{-p_1} X_2^{-p_2} \cdots X_m^{-p_m}.
\]

(23)

Table 1 presents the four carbon fluxes present in the pre-industrial state of the Anderies et al. model, and their corresponding rate functions. Furthermore, the last column lists their respective target power-law approximation. The last two functions, $a_m A_2$ and $a_m \beta A_3$, are already in the desired format and are thus, kept as is. To compute for the kinetic orders (and rate constants), we apply (23). By taking the parameter values used in [11] but with $\alpha = 0$, and assuming the initial values to be $A_1 = 2850/4500$, $A_2 = 750/4500$ and $A_3 = 900/4500$ (as in [1]), the ODE system in [22] reaches the following steady state: $A_1 = 0.7$, $A_2 = 0.15$ and $A_3 = 0.15$.

The algebraic calculations are implemented in Mathematica, with codes shown in Figure 2. When $\alpha = 0$ (i.e., the human off-take term vanishes),

\[
p_1 = p_2 = \frac{2A_1 - k}{A_1 - k}.
\]
Table 1. Power-law approximation of the process rates.

| Carbon Flux Function | Power-law approx. |
|----------------------|-------------------|
| $A_2 \rightarrow A_1$ | $K_1 = r_{A_1} P(t) A_1 \left[ 1 - \frac{A_1}{K_1} \right] k_1 A_1^{q_1_1} A_2^{q_1_2}$ |
| $A_1 \rightarrow A_2$ | $K_2 = r_{A_2} R(t) A_1 \left[ 1 - \frac{A_1}{K_1} \right] + \alpha A_1 k_2 A_1^{q_2_1} A_2^{q_2_2}$ |
| $A_2 \rightarrow A_3$ | $K_3 = a_m A_2$ |
| $A_1 \rightarrow A_2$ | $K_4 = a_m \beta A_3$ |

For the power-law approximation, we choose values close to the equilibrium point as operating point: $A_1 = 0.69, A_2 = 0.155$ and $A_3 = 0.155$. Consequently, we obtain

$$p_1 = -68, \quad p_2 = -68, \quad q_1 = 0.580148, \quad q_2 = 0.910864. \quad (24)$$

Fig. 2. Mathematica codes.