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S-invariant Termwise Addition of Reactions Via Reaction Vector Multiples (STAR-RVM) Transformation

Daryl M. Magpantay

College of Arts and Sciences, Batangas State University - The National Engineering University, Batangas City, Batangas, Philippines

Abstract. Interest in connecting Chemical Reactions Network Theory (CRNT) and evolutionary game theory (EGT) arise viewing the tools of network in the analysis of evolutionary games. Here, the evolution of population species is studied as a biological phenomenon and describing the rate of such changes through a replicator system becomes a focus. A set of polynomial kinetics (POK) may then be introduced for the realization of this replicator system and this is based on the polynomial payoff functions defined in the game. These polynomial kinetics result in polynomial dynamical systems of ordinary differential equations, which are used in analyzing strategies that prove beneficial under certain conditions. From the CRNT point of view, it now becomes interesting to study a superset of POK, which we call poly-PL kinetics (PYK). This set is formed by getting nonnegative linear combinations of power law functions. Thus, PYK contains the set PLK of power law kinetics as mono-PL kinetics with coefficient 1. Seeing this connection between CRNT and EGT and what are known about power law kinetics, we take an interest in studying PYK systems. This paper aims to analyze different ways of transforming PYK to PLK in order to explore some approaches for CRNT analysis of PYK systems. Specifically, we study a network structure-oriented transformations using the S-invariant term-wise addition of reactions (STAR) Via Reaction Vector Multiples (RVM) that transform PYK to PLK systems.

2020 Mathematics Subject Classifications: 92

Key Words and Phrases: Chemical Reactions Network Theory, power law kinetics, Reaction Vector Multiples, mono-PL kinetics

1. Introduction

The study of evolutionary game theory (EGT) revolves around dynamics that describe the spread of successful strategies in a population of various species. EGT models how individuals or populations change their strategy over time based on payoff comparisons. One important game dynamics that is mostly studied is the replicator equation. This

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Email address: `daryl.magpantay@g.batstate-u.edu.ph` (D. Magpantay)

equation allows the reproduction success technically known as fitness function to incorporate the distribution of the finitely many species in the population. With this property, a replicator equation captures the essence of natural selection so that traits that favor survival and reproduction (i.e., having higher fitness or reproductive success) contribute to increase in size over generations. Payoffs are translated as fitness so that over time the change in the frequency of a strategy in a large, well-mixed population is described through the replicator equation. This rate is described as the product of the proportion of this species and the difference between its expected payoff and the average payoff of the population [3].

Veloz et al. [9] proposed a manner of analyzing the dynamics of EGT games using chemical reaction network. From this vantage point, an encounter between two species is treated as a reaction that results in a gain or loss (i.e. payoff) for each species. They introduced a set of polynomial kinetics for the realization of replicator system-based evolutionary games with polynomial payoff functions (mostly linear functions). The proposed analysis allows for the application of Chemical Reactions Network Theory (CRNT). CRNT is an area of applied mathematics that attempts to model the behavior of real world chemical systems. It aims to understand connections between network structure and system dynamics with mathematical methods from graph theory, linear algebra, group theory and the theory of ordinary differential equations.

Results from Mendoza et al. [7] included the subset of sums of power law kinetics. A particular interesting family of kinetics of this type is the polynomial kinetic system where all exponents are non-negative integers, which is a sum of monomials with real coefficients. The consideration of the superset called poly-PL kinetics (PYK), i.e. of real exponents instead of just non-negative integers, came from the observation that “sums of power law functions” occurred in power law approximations of some carbon cycle models in [6]. Thus, PYK contains the set PLK of power law kinetics as mono-PL kinetics with coefficient 1. With this relationship and available results in PLK, we are motivated to analyze PYK systems in CRNT setting. This leads us to an interest in finding different ways to transform PYK to PLK.

The contribution of this paper is to explore some approaches for CRNT analysis of PYK systems specifically via dynamic equivalence to power kinetic systems using S-invariant Term-wise Addition of Reactions (STAR) approach. A STAR method introduces additional different reaction(s) for each of the identical reaction vectors in the sum.

2. Preliminaries

2.1. Basic Concepts on Chemical Reaction Network Theory (CRNT)

We begin by defining concepts related to chemical reaction network. These were taken from the PhD thesis of Boros [2].

Definition 1. *Let $\mathscr{S}$ be a non-empty finite set of* ***chemical species****. A* ***chemical complex*** *is a linear combination of the species with non-negative integer coefficients called*

stoichiometric coefficients. *The set of complexes is denoted by* $\mathscr{C}$. *We reserve* m *to denote the number of species and* n *to denote the number of complexes.*

A complex is called **monospecies** if it consists of only one species, i.e. of the form kA_i, k a non-negative integer and A_i a species. It is called **monomolecular** if $k = 1$, and is identified with the **zero complex** for $k = 0$. A zero complex represents the "outside" of the system studied, from which chemicals can flow into the system at a constant rate and to which they can flow out at a linear rate (proportional to the concentration of the species). In biological systems, the "outside" also stands for the degradation of a species. An **inflow reaction** is a reaction with source "0" and an **outflow reaction** is a reaction with a monomolecular complex as source and the zero complex as target.

Definition 2. *The* ***set of reactions*** $\mathscr{R}$ *is a non-empty subset of* $\mathscr{C} \times \mathscr{C}$ *such that*

(a) $(y, y) \notin \mathscr{R}$, *for all* $y \in \mathscr{C}$; *and*

(b) for each $y \in \mathscr{C}$, *there exists a* $y' \in \mathscr{C}$ *such that* $(y', y) \in \mathscr{R}$ *or such that* $(y, y') \in \mathscr{R}$.

We denote r *as* $|\mathscr{R}|$ *or the number of reactions.*

For each $(y, y') \in \mathscr{R}$ we say that a complex y reacts to complex y'. Also, we can write $y \to y'$ in place of (y, y'). In this paper, the notations (y, y') or $y \to y'$ are used interchangeably and we say that y is the **reactant complex** and y' is the **product complex** of the reaction.

We now formally define a chemical reaction network.

Definition 3. *A* ***chemical reaction network (CRN)*** *is a triple* $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ *of three non-empty finite sets, where* $\mathscr{S}$ *is the set of chemical species,* $\mathscr{C}$ *is the set of chemical complexes, and* $\mathscr{R}$ *is the set of reactions.*

Example 1. Let $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ be a chemical reaction network such that

$\mathscr{S} = \{A_1, A_2, A_3, A_4\}$

$\mathscr{C} = \{2A_1, A_2 + A_3, A_3, 3A_4\}$

$\mathscr{R} = \{2A_1 \to A_3, A_2 + A_3 \to A_3, A_3 \to A_2 + A_3, 3A_4 \to A_2 + A_3, 2A_1 \to 3A_4\}$ or

$\mathscr{R} = \{(2A_1, A_3), (A_2 + A_3, A_3), (A_3, A_2 + A_3), (3A_4, A_2 + A_3), (2A_1, 3A_4)\}$

As observed, $m = 4$, $n = 4$ and $r = 5$.

2.2. Connectivity in a CRN

We first recall some basic concepts of graph theory. Two vertices y and y' are *connected* if there is a path between them, i.e. a sequence of adjacent vertices $y = y_1, y_2, \cdots y_n = y'$. They are *strongly connected* if there is a directed path between y and y' and vice versa. Connected and strongly connected are equivalence relations, and the equivalence classes are called *connected components* and *strong connected components*, respectively. Each connected component is clearly the disjoint union of strong connected components.

Connectivity in a digraph that is applied to CRNs is traditionally called a **linkage class** in CRNT. We formally define it as follows:

Definition 4. *A **linkage class** of a CRN is a maximal weakly connected subgraph of its reaction graph. A **strong linkage class** is a maximal strongly connected subgraph of the reaction graph. A **terminal strong linkage class** is a strong linkage class containing no complex that reacts to a complex belonging to a different strong linkage class.*

Example 2. Note that for Example 1 we have:

1 linkage class: $\{2A_1, A_3, A_2 + A_3, 3A_4\}$;

3 strong linkage classes: $\{A_3, A_2 + A_3\}$, $\{2A_1\}$ and $\{3A_4\}$; and

1 terminal strong linkage class: $\{A_3, A_2 + A_3\}$.

We denote the number of linkage classes with ℓ , that of the strong linkage classes with $s\ell$, and that of terminal strong linkage classes with t. Clearly, $\ell \leq t \leq s\ell$. There are two types of terminal strong linkage classes in a CRN: cycles and singletons (which are called terminal points).

Definition 5. *A CRN is called:*

*i) **point terminal** if $t = n - n_r$;*

*ii) **weakly reversible** if $s\ell = \ell$, i.e. every linkage class is a strong linkage class; and*

*iii) **t-minimal** if $t = \ell$, i.e. every linkage class contains exactly one terminal strong linkage class.*

Remark 1. *We denote by t_c the number of cycle-terminal classes and t_p the number of point-terminal classes. Then $t = t_c + t_p$. Note also that $n - n_r = t_p = t - t_c$. A CRN is cycle-terminal if $t_p = 0$ (i.e. $n = n_r$), point-terminal if $t_c = 0$ (i.e. $t = n - n_r$) and point- and cycle-terminal otherwise (i.e. $t_p > 0$ and $t_c > 0$ or equivalently, $t > n - n_r$).*

Example 3. As observed in Example 1, $t = 1$ and $n - n_r = 4 - 4 = 0$. This implies that the network is not point terminal. Also, $s\ell = 3 \neq 1 = \ell$. Hence, the network is not weakly reversible. But, $t = 1 = \ell$. Thus, the network is t-minimal.

A network in the form of a simple cycle is an example of a weakly reversible network.

The next proposition shows that the set of nonbranching digraphs is a subset of the set of t-minimal digraphs.

Proposition 1. *If a digraph is nonbranching, then it is t-minimal.*

Proof. Suppose a digraph is not t-minimal. That is, there is a connected component with at least two terminal strong components T, T'. If y is in T and y' in T', then there is an (undirected) path from y to y', with the first arc pointing into T and the last arc pointing into T'. Clearly, there must at least one vertex v with $d^+(v) \geq 2$, contradicting the nonbranching hypothesis.

2.3. Deficiency of a CRN

A central concept of the theory of chemical reaction networks is the deficiency of the CRN. Shinar and Feinberg [8] describe the "deficiency philosophy" as follows: The deficiency of a reaction network is an integer index that assumes a non-negative value. Loosely speaking, the deficiency measures the amount of linear independence among the reactions of the network. The lowest value that the deficiency can assume, which is zero, is associated with the highest possible extent of linear independence among the individual reactions, consistent with the network's structure as a directed graph. The higher the deficiency, the lower the extent of linear independence. We formally define the deficiency of a CRN as follows:

Definition 6. *The* ***deficiency of a CRN*** *is the integer* $\delta = n - \ell - s$.

Example 4. In Example 1, observe that $n = 4$, $\ell = 1$ and $s = 3$. With this, the deficiency of the network $\delta = n - \ell - s = 4 - 1 - 3 = 0$.

By relating deficiency to linear maps defined from a CRN, we have the following proposition which is a classical result. One can refer to [4] but we provide its proof for the convenience of the reader.

Proposition 2. *The deficiency* δ *is equal to* $dim(kerY \cap Im\ I_a)$.

Proof. It follows from basic dimensional considerations that

$$dim(ker(Y\ I_a)) = dim(ker(I_a)) + dim(ker(Y) \cap Im(I_a)).$$

From the rank-nullity theorem, we have

$$dim(ker(Y\ I_a)) = r - dim(Im(Y\ I_a)) = r - s.$$

The rank of I_a corresponds to the number of complexes minus the number of linkage classes, so that

$$dim(Im(I_a)) = n - \ell.$$

It follows that

$$dim(ker(I_a)) = r - (n - \ell) = r + \ell - n$$

It implies that

$$\begin{aligned} & dim(ker(Y) \cap Im(I_a)) \\ = \; & dim(ker(Y\ I_a)) - dim(ker(I_a)) \\ = \; & (r - s) - (r + \ell - n) \\ = \; & n - \ell - s \\ = \; & \delta. \end{aligned}$$

2.3.1. Terminality and Reactant Diversity

The terminality of a network is the non-negative integer $\tau(\mathscr{N}) = t - \ell$. We now introduce useful partition of networks with respect to terminality:

Definition 7. *A CRN is of type* ***terminality bounded by deficiency (TBD)*** *if* $t - \ell \leq \delta$. *Otherwise, it is of type* ***terminality not deficiency-bounded (TND)****, i.e.* $t - \ell > \delta$.

Definition 8. *A CRN has* ***low reactant diversity (LRD)*** *if* $n_r < s$,*. Otherwise it has* ***sufficient reactant diversity (SRD)****. An SRD network has* ***high reactant diversity (HRD)*** *or* ***medium reactant diversity (MRD)*** *if* $n_r > s$ *or* $n_r = s$*, respectively.*

Example 5. Going back to the Example 1, we have $t - \ell = 1 - 1 = 0 = \delta$ and $n_r = 4 > 3 = s$. Hence, the CRN is of type terminality bounded by deficiency (TBD) and has sufficient reactant diversity (SRD).

The next proposition provides the initial positioning of reactant diversity in the CRN landscape:

Proposition 3. *A TBD network is an SRD network.*

Proof. Since the network is TBD, $t - \ell \leq \delta$. This implies that $(n - n_r) - \ell \leq n - s - \ell$. Hence, $n - n_r \leq n - s$ and so $n_r \geq s$.

Corollary 1. *A t-minimal network is an SRD network.*

For a point terminal networks, we obtain the following equivalences:

Proposition 4. *For a point terminal CRN, a network is SRD if and only if it isTBD.*

Proof. Since the network is SRD, $n_r \geq s$. With this, $(n - n_r) - \ell \leq n - s - \ell$. Thus, $t - \ell \leq \delta$.

2.4. Reactant Subspace

In this section, our focus was on the set of reactant complexes $\rho(\mathscr{R})$ and its cardinality n_r. The following was the linear space generated by $\rho(\mathscr{R})$.

Definition 9. *The **reactant subspace** R is the linear space in $\mathbb{R}^{\mathscr{S}}$ generated by the reactant complexes, i.e. $\langle \rho(\mathscr{R}) \rangle$. The value $q := \dim R$ is called the **reactant rank** of the network.*

Remark 2. *We denote dim R by "q" (since "r" is already reserved for the number of reactions). We also denote dim Im Y by "c" (since Im Y consists precisely of the network's complexes embedded in $\mathbb{R}^{\mathscr{S}}$).*

Example 6. As per Example 1, the reactant subspace $R = \langle \{2A_1, A_2 + A_3, A_3, 3A_4\} \rangle$. With this, the reactant rank is $q = 4$.

The relationship of the reactant rank to the network's rank is important in the study of the reactant subspace and we introduce some relevant concepts here.

Definition 10. *The **rank difference** $\Delta(\mathscr{N})$ is equal to $s - q$. The network has **high reactant rank (HRR)** if $\Delta(\mathscr{N})$ is negative, **medium reactant rank (MRR)** if it is zero and **low reactant rank (LRR)** if it is positive.*

Example 7. Referring to Example 1, observe that the rank difference $\Delta(\mathscr{N}) = s - q = 3 - 4 = -1$. Thus, the network has high reactant rank (HRR).

In the previous discussion, we introduce the deficiency of the network. We now introduce deficiency focusing on the reactant complexes. This concept was introduced by Arceo et al [1].

Definition 11. *The **reactant deficiency** $\delta_\rho := n_r - q$, i.e., the difference between the number of reactant complexes and the reactant rank q.*

Example 8. The reactant deficiency of the network in Example 1 is $\delta_\rho := n_r - q = 4 - 4 = 0$.

2.5. Poly-PL Kinetic Systems

In this section, we introduce a more general definition of a kinetics. We begin with the definition and basic properties of a chemical kinetic system (CKS).

A kinetics for a CRN is an assignment of a rate function to each reaction in the network. This is defined formally below.

Definition 12. *A **kinetics** of a CRN $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ is an assignment of a rate function $K_{ij} : \Omega_K \to \mathbb{R}_{\geq}$ to each reaction $(i, j) \in \mathscr{R}$, where Ω_K is a set such that $\mathbb{R}^{\mathscr{S}}_{>} \subseteq \Omega_K \subseteq \mathbb{R}^{\mathscr{S}}_{\geq}$, and*

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

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

The above definition is adopted from the paper of Wiuf & Feliu [10]. However, in this paper, we use simpler definition of CKS as follows:

Definition 13. *A* ***chemical kinetics*** *is a kinetics satisfying the positivity condition:*

For each reaction $(i, j) \in \mathscr{R}, K_{ij}(c) > 0$ *if and only if supp* $i \subset$ *supp* c*, where* $c \in \Omega_K$.

Remark 3. *(Feinberg, 1987) The "positivity condition" requires that the rate function* K_{ij} *of the reaction* $i \to j$ *proceeds at a nonzero rate at a specified composition precisely when all species in the reactant complex* i *are present in this composition. Note that the notation supp* c *refers to the set of species in the CRN that have nonzero concentrations at composition* c*. On the other hand, supp* i *pertains to the set of species in the complex* i *i.e., these are the "ingredients" required for the reaction* $i \to j$ *to happen. Hence, by supp* $i \subset$ *supp* c*, we mean that at composition* c*, all ingredients needed for the occurrence of the reaction* $i \to j$ *are available.*

A chemical kinetics gives rise to two closely related objects: the species formation rate function (SFRF) and the associated ODE systems:

Definition 14. *The* ***species formation rate function (SFRF)*** *of CKS is the vector field*

$$f(x) = NK(x) = \sum_{y \to y'} K_{y \to y'}(x)(y' - y).$$

where N *is the stoichiometric matrix. The equation* $\dot{c} = f(c)$ *is the* ***ODE*** *or* ***dynamical system*** *of the CKS.*

Example 9. Refering to Example 1, the dynamical system of the CKS is

$$\dot{c} = NK(c) = \begin{bmatrix} -2 & 0 & 0 & 0 & -2 \\ 0 & -1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 & 3 \end{bmatrix} \begin{bmatrix} K_{2A_1 \to A_3} \\ K_{A_2 + A_3 \to A_3} \\ K_{A_3 \to A_2 + A_3} \\ K_{3A_4 \to A_2 + A_3} \\ K_{2A_1 \to 3A_4} \end{bmatrix}.$$

Here, $K(X)$ is called the kinetic vector. We will assume that the ODE system above is under **power law kinetics (PLK)** which have the form

$$K_i(x) = k_i \prod_{j=1}^{m} x^{F_{ij}} \quad where\ 1 \le i \le r$$

with $k_i \in \mathbb{R}_+$ and $F_{ij} \in \mathbb{R}$. Power law kinetics is defined by an $r \times m$ matrix $F = [F_{ij}]$, called the **kinetic order matrix**, and vector $k \in \mathbb{R}^r$, called the **rate vector**. A particular example of power law kinetics is the well-known mass action kinetics where the kinetic order matrix consists of stoichiometric coefficients of the reactants. In Example 1, we assume power law kinetics so that the kinetic order matrix is

$$F = \begin{array}{c} \\ \\ \\ \\ \\ \end{array}\begin{array}{cc} \begin{array}{cccc} A_1 & A_2 & A_3 & A_4 \end{array} & \\ \left[\begin{array}{cccc} f_{11} & 0 & 0 & 0 \\ 0 & f_{22} & f_{32} & 0 \\ 0 & 0 & f_{33} & 0 \\ 0 & 0 & 0 & f_{44} \\ f_{15} & 0 & 0 & 0 \end{array}\right] & \begin{array}{c} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \end{array} \end{array}$$

where $f_{ij} \in \mathbb{R}$.

Poly-PL kinetics (PYK) are kinetic systems consisting of non-negative linear combinations of power law functions. This set contains the set PLK of power law kinetics as "mono-PL kinetics with coefficient 1". Like PLK, the definition domain of PYK is the positive orthant $\mathbb{R}^m_>$. However, for subsets, this may be extended to the whole non-negative orthant $\mathbb{R}^m_\geq$. Clearly, PYK and PLK generate the same sets of SFRFs, the power law dynamical systems (or GMA systems in BST terminology).

After setting the standard ordering of species $X_1, \ldots, X_m$, we have the following definition:

Definition 15. *A kinetics $K : \mathbb{R}^m_> \to \mathbb{R}^r$ is a* ***poly-PL kinetics*** *if*

$$K_i(x) = k_i(a_{i,1}x^{F_{i,1}} + \ldots + a_{i,j}x^{F_{i,j}}) \quad \textit{where } 1 \leq i \leq r \tag{1}$$

written in lexicographic order with $k_i \in \mathbb{R}_+$, $F_{i,j}, a_{i,j} \in \mathbb{R}^m$ and $1 \leq j \leq h_i$ (where h_i is the number of terms in reaction i). Power-law kinetics is defined by $r \times m$ matrices $F_{i,k} = [F_{ij}]$, called the ***kinetic order*** *matrices, vectors $k = [k_i]$ called the* ***rate vector*** *and $a_{i,j} \in \mathbb{R}^r_>$ called the* ***poly-rate vectors****.*

Example 10. *For $(\mathscr{N}, K)$ with $\mathscr{S} = \{X, Y\}$ and $\mathscr{R} = \{r : X \to 2X, r' : 2X \to 5X + Y\}$, let the poly-PL kinetics be given by :*

$$K_1(X, Y) = k_1(2XY + 0.5Y^2) \textit{ and } K_2(X, Y) = k_2(0.75X^2Y + X^3)$$

where k_1, k_2 are rate constants. The kinetic order matrices are

$$F_{1,k} = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix}; \textit{ and } F_{2,k} = \begin{bmatrix} 2 & 1 \\ 3 & 0 \end{bmatrix}$$

with the kinetic order vector

$$k = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix}.$$

2.6. STAR Transformations of Chemical Kinetic Systems

Now, we introduce the concept of transformation of chemical kinetic system as a special kind of dynamic equivalence. We begin with a formal definition of dynamic equivalence of chemical kinetic systems.

Definition 16. *A chemical kinetic system* $(\mathscr{N}^*, K^*)$ *is* ***dynamically equivalent*** *to* $(\mathscr{N}, K)$ *if:*

(i) $\mathscr{N}^*$ *and* $\mathscr{N}$ *have the same set of species, i.e.* $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ *and* $\mathscr{N}^* = (\mathscr{S}, \mathscr{C}^*, \mathscr{R}^*)$

(ii) N^* *and* N *are their respective stoichiometric matrices, then their SFRF´s (vector fields) coincide, i.e.* $f^* = N^*K^* = NK = f$.

Condition (i) implies that additional complexes and reactions do not affect the said equivalence. As for condition (ii), an immediate necessary condition for dynamic equivalence is the coincidence of their kinetic subspaces as shown in the following proposition:

Proposition 5. *If* $(\mathscr{N}^*, K^*)$ *is dynamically equivalent to* $(\mathscr{N}, K)$*, then their kinetic subspaces* K^* *and* K *are equal.*

Proof. Since $(\mathscr{N}^*, K^*)$ is dynamically equivalent to $(\mathscr{N}, K)$, $f^* = f$. Hence,

$$\begin{aligned} Im\ f^* &= Im\ f \\ span(Im\ f^*) &= span(Im\ f) \\ K^* &= K. \end{aligned}$$

We tolerate the use of K and K^* for two different meanings (kinetics and kinetic subspace) since it is usually clear from the context which one is referred to.

We know the fact that the kinetic subspace is contained in the stoichiometric subspace S for any chemical kinetic system but in general, they may not coincide (for example, for MAK systems with $t - \ell > \delta$). Our new concept requires that this structural property holds:

Definition 17. *A chemical kinetic system* $(\mathscr{N}^*, K^*)$ *is a* ***transformation*** *of* $(\mathscr{N}, K)$ *if:*

i) $(\mathscr{N}^*, K^*)$ *is dynamically equivalent to* $(\mathscr{N}, K)$ *and*

ii) $S^* = S$.

This will be the basis of the transformations that are introduced throughout this chapter.

2.7. STAR transformation: definition and basic properties

STAR (S-invariant Termwise Addition of Reactions) is a network structure-oriented approach to poly-PL Kinetics based on the following basic observation: for the rate function $K_i(x)$ and for a reaction $r_i : y_i \to y_i'$ in a PYK system $(\mathscr{N}, K)$ with $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ we have

$$K_i(x) = k_i(a_{i1}M_{i1} + \ldots + a_{ih}M_{ih})(y_i' - y_i) = k_i a_{i1} M_{i1}(y_i' - y_i) + \ldots + k_i a_{ih} M_{ih}(y_i' - y_i) \quad (2)$$

where M_{ij} are the h power law functions for the i-th reaction.

A STAR method introduces additional different reaction(s) for each of the h identical reaction vectors $y_i' - y_i$ in the sum. This enlarges the sets of reactions and complexes, so the new CRN $\mathscr{N}^* = (\mathscr{S}, \mathscr{C}^*, \mathscr{R}^*)$ and new kinetics $K^* : \mathbb{R}^{\mathscr{S}}_{>} \to \mathbb{R}^{\mathscr{R}^*}$ are constructed.

Remark 4. *When the poly-PL kinetics do not have the same number of terms, one simply uses the same "trick" of replacing the last term of the shorter function with* $(h - h' + 1)$ *copies of* $\frac{1}{h-h'+1}$ *of that term.*

Illustration 1. *Suppose the following are the poly-PL kinetics of a network:*

$$K_1(X, Y) = k_1(2X^3Y + X^2Y^2 + 4XY^2 + 0.5Y^3)$$

$$K_2(X, Y) = k_2(5X^4Y^2 + 6XY^3).$$

It is equvalent to

$$K_1(X, Y) = k_1(2X^3Y + X^2Y^2 + 4XY^2 + 0.5Y^3)$$

$$K_2(X, Y) = k_2(5X^4Y^2 + 2XY^3 + 2XY^3 + 2XY^3).$$

Notice that $\mathscr{N}$ and $\mathscr{N}^*$ have the same set of species as one of requirements to be dynamically equivalent. Since it is S-invariant and it is a transformation, this assures the equality of the stoichiometric subspace S of the original network to the stoichiometric subspace S^* of the network produced by adding complexes and reactions. This implies $s = dim\ S = dim\ S^* = s^*$.

Aside from these observations, we have the following properties for any STAR method:

Proposition 6. *Let* $\mathscr{N}^* = (\mathscr{S}, \mathscr{C}^*, \mathscr{R}^*)$ *be a STAR transform of* $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$. *Then* $|\mathscr{R}^*| = hr$ *and* $|\mathscr{C}^*| \leq hn$.

Proof. For the first part, since STAR method introduces an additional different reaction for each of the h identical reaction vectors $y_i' - y_i$ in the sum, the claim follows immediately from (2) and from the fact that hn is the maximum number of complexes (i.e. when these are all different) for hr reactions.

Remark 5. *Observe that* $K^*_{ij} = k^*_{ij} M_{ij}$, *with* $k^*_{ij} = k_i a_{ij}$, *is the kinetic function of the reaction* R_{ij} *corresponding to the reaction vector* $(y_i' - y_i)$. *The stoichiometric matrix* N^*

becomes an $m \times hr$ *matrix, and usually the reaction vector of the reaction* r_i *are just replicated* h *times.*

Let the reaction vector $y_i' - y_i = (c_{i1}, c_{i2}, \dots, c_{im})$. By the remark above, we have

$$N^* = \begin{array}{ccccccccccccc|c} R_{11} & R_{12} & \dots & R_{1h} & R_{21} & R_{22} & \dots & R_{2h} & \dots & R_{r1} & R_{r2} & \dots & R_{rh} & \\ \hline c_{11} & c_{11} & \dots & c_{11} & c_{21} & c_{21} & \dots & c_{21} & \dots & c_{r1} & c_{r1} & \dots & c_{r1} & A_1 \\ c_{12} & c_{12} & \dots & c_{12} & c_{22} & c_{22} & \dots & c_{22} & \dots & c_{r2} & c_{r2} & \dots & c_{r2} & A_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ c_{1m} & c_{1m} & \dots & c_{1m} & c_{2m} & c_{2m} & \dots & c_{2m} & \dots & c_{rm} & c_{rm} & \dots & c_{rm} & A_m \end{array}$$

and

$$K^* = \begin{bmatrix} K_{11}^* \\ K_{12}^* \\ \vdots \\ K_{1h}^* \\ K_{21}^* \\ K_{22}^* \\ \vdots \\ K_{2h}^* \\ \vdots \\ K_{r1}^* \\ K_{r2}^* \\ \vdots \\ K_{rh}^* \end{bmatrix}.$$

Hence,

$$N^*K^* = \begin{bmatrix} c_{11}K_{11}^* + c_{11}K_{12}^* + \dots + c_{11}K_{1h}^* + c_{21}K_{21}^* + c_{21}K_{22}^* + \dots + c_{21}K_{2h}^* + \dots + c_{r1}K_{r1}^* + c_{r1}K_{r2}^* + \dots + c_{r1}K_{rh}^* \\ c_{12}K_{11}^* + c_{12}K_{12}^* + \dots + c_{12}K_{1h}^* + c_{22}K_{21}^* + c_{22}K_{22}^* + \dots + c_{22}K_{2h}^* + \dots + c_{r2}K_{r1}^* + c_{r2}K_{r2}^* + \dots + c_{r2}K_{rh}^* \\ \vdots \\ c_{1m}K_{11}^* + c_{1m}K_{12}^* + \dots + c_{1m}K_{1h}^* + c_{2m}K_{21}^* + c_{2m}K_{22}^* + \dots + c_{2m}K_{2h}^* + \dots + c_{rm}K_{r1}^* + c_{rm}K_{r2}^* + \dots + c_{rm}K_{rh}^* \end{bmatrix}$$

$$= \begin{bmatrix} c_{11}(K_{11}^* + K_{12}^* + \dots + K_{1h}^*) + c_{21}(K_{21}^* + K_{22}^* + \dots + K_{2h}^*) + \dots + c_{r1}(K_{r1}^* + K_{r2}^* + \dots + K_{rh}^*) \\ c_{12}(K_{11}^* + K_{12}^* + \dots + K_{1h}^*) + c_{22}(K_{21}^* + K_{22}^* + \dots + K_{2h}^*) + \dots + c_{r2}(K_{r1}^* + K_{r2}^* + \dots + K_{rh}^*) \\ \vdots \\ c_{1m}(K_{11}^* + K_{12}^* + \dots + K_{1h}^*) + c_{2m}(K_{21}^* + K_{22}^* + \dots + K_{2h}^*) + \dots + c_{rm}(K_{r1}^* + K_{r2}^* + \dots + K_{rh}^*) \end{bmatrix}$$

$$= \begin{bmatrix} c_{11}K_1 + c_{21}K_2 + \dots + c_{r1}K_r \\ c_{12}K_1 + c_{22}K_2 + \dots + c_{r2}K_r \\ \vdots \\ c_{1m}K_1 + c_{2m}K_2 + \dots + c_{rm}K_r \end{bmatrix}$$

$$= \begin{bmatrix} c_{11} & c_{21} & \cdots & c_{r1} \\ c_{12} & c_{22} & \cdots & c_{r2} \\ \vdots & & & \\ c_{1m} & c_{2m} & \cdots & c_{rm} \end{bmatrix} \begin{bmatrix} K_1 \\ K_2 \\ \vdots \\ K_r \end{bmatrix} = NK$$

Thus, $f^* = N^*K^* = NK = f$ and so $(\mathscr{N}^*, K^*)$ is dynamically equivalent to $(\mathscr{N}, K)$ under STAR transformation.

3. The S-invariant Termwise Addition of Reactions Via Reaction Vector Multiples (STAR-RVM) Transformation

In this section, we introduce the first method of STAR transformation. Also, we identify and compare the network numbers and discuss the variant and invariant CRN properties.

3.1. Definition and Some illustrative examples

In STAR transformations, new reactions and complexes are added. There are various ways of constructing a CRN from these. One method is by using reaction vector multiples described as follows:

Definition 18. *Let $\mathscr{N} = (\mathscr{S}, \mathscr{C}, \mathscr{R})$ be a CRN and $y \to y' \in \mathscr{R}$ with $y' - y = (c_1, \ldots, c_k)$ satisfying the condition that either $c_i \geq 0$ or $c_i \leq 0$ for all $i = 1, \ldots, k$. The **S-invariant Termwise Addition of Reactions Via Reaction Vector Multiples (STAR-RVM)** transform, $(\mathscr{N}^*, K^*)$, for each reaction $y \to y'$ having poly-PL kinetics $K(x) = \sum_{j=1}^{h} a_j P_j$ proceeds as follows:*

(i) when $c_i \geq 0$ for all $i = 1, \ldots, k$, define the additional complexes and reactions

$$y \to y' \to y' + (y' - y) \to y' + 2(y' - y) \to \cdots y' + (h-1)(y' - y)$$

with corresponding kinetics $P_1^*, P_2^*, \ldots, P_h^*$;

(ii) when $c_i \leq 0$ for all $i = 1, \ldots, k$, define the additional complexes and reactions

$$y + (h-1)(y - y') \to \cdots \to y + 2(y - y') \to y + (y - y') \to y \to y'$$

with corresponding kinetics $P_h^*, \ldots, P_2^*, P_1^*$

where $P_j^* = a_j P_j$, $1 \leq j \leq h$.

Example 11. For $(\mathscr{N}, K)$ with $\mathscr{S} = \{X, Y\}$ and $\mathscr{R} = \{r : X \to 2X, r' : 2X \to 5X + Y\}$, let the poly-PL kinetics be given by :

$$K_r(X,Y) = k(2XY + 0.5Y^2) \qquad K_{r'}(X,Y) = k'(0.75X^2Y + X^3)$$

where k, k' are rate constants.

The reaction vector for reaction r is $2X - X = X$ and for reaction r' is $5X + Y - 2X = 3X + Y$. Generating STAR-RVM transform, we have $(\mathscr{N}^*, K^*)$ where $\mathscr{S} = \{X, Y\}$ and $\mathscr{R}^* = \{r : X \rightarrow 2X, r^* : 2X \rightarrow 3X, r' : 2X \rightarrow 5X + Y, r'^* : 5X + Y \rightarrow 8X + 2Y\}$. The kinetic functions are as folows:

$$K^*_r(X,Y) = 2kXY = k^*XY \qquad K^*_{r^*}(X,Y) = 0.5kY^2 = k^{**}Y^2$$
$$K^*_{r'}(X,Y) = 0.75k'X^2Y = k'^*X^2Y \qquad K^*_{r'^*}(X,Y) = k'X^3 = k'^{**}X^3$$

Example 12. For $(\mathscr{N}, K)$, with $\mathscr{S} = \{X, Y\}$ and $\mathscr{R} = \{r_1 : 2X + 2Y \rightarrow X + Y, r_2 : X + Y \rightarrow 2X + Y, r_3 : 2X + Y \rightarrow 2X + 2Y\}$. Let the poly-PL kinetics be given by (k_1, k_2, k_3 are as usual the rate constants):

$$K_{r_1}(X,Y) = k_1(0.2XY + 5Y^2) \qquad K_{r_2}(X,Y) = k_2(0.3X^2 + 2X^3Y)$$
$$K_{r_3}(X,Y) = k_3(2.5X + 3Y^3)$$

Generating STAR-RVM transform, we have $(\mathscr{N}^*, K^*)$ where $\mathscr{S} = \{X, Y\}$ and $R^* = \{r_1 : 2X + 2Y \rightarrow X + Y, r_1^* : 3X + 3Y \rightarrow 2X + 2Y, r_2 : X + Y \rightarrow 2X + Y, r_2^* : 2X + Y \rightarrow 3x + Y, r_3 : 2X + Y \rightarrow 2X + 2Y, r_3^* : 2X + 2Y \rightarrow 2X + 3Y\}$. The kinetic functions are as folows:

$$K^*_{r_1}(X,Y) = 0.2k_1XY = k_1^*XY \qquad K^*_{r_1^*}(X,Y) = 5k_1Y^2 = k_1^{**}Y^2$$
$$K^*_{r_2}(X,Y) = 0.3k_2X^2 = k_2^*X^2 \qquad K^*_{r_2^*}(X,Y) = 2k_2X^3Y = k_2^{**}X^3Y$$
$$K^*_{r_3}(X,Y) = 2.5k_3X = k_3^*X \qquad K^*_{r_3^*}(X,Y) = 3k_3Y^3 = k_3^{**}Y^3$$

3.2. A comparison of network numbers

The network numbers of a CRN refers to the number of species, complexes, reactant complexes, reactions, linkage classes, strong linkage classes and terminal strong lingkage classes. It also includes the rank, reactant rank, rank difference, deficiency and reactant deficiency of the network. It provides different descriptions of a network and basis of comparison to the other networks.

For the STAR-RVM method, we compare the network numbers of the original and the transformed network. These are reflected on Table 3.1.

Since we have the same set of species, $m^* = m$. Note that the number of possible additional complexes is $r(h-1)$. This means that the maximum number of complexes in $\mathscr{N}^*$ is $r(h-1) + n$ since it will depends on whether all additional complexes are unique compared to the original complexes and within the set. The same may be said about the reactant complexes of the two networks.

As part of the properties of STAR transformation shown in Table 3.1, we have $|\mathscr{R}^*| = r^* = hr$ and $s^* = s$. Observe that on the construction using STAR-RVM method, no additional linkage class is produced. However, it is possible that original number of linkage

Table 1: Network Numbers of STAR-RVM Transform

Network Number	**Value/Bounds**
Number of species	$m^* = m$
Number of complexes	$n \leq n^* \leq r(h-1) + n$
Number of reactant complexes	$n_r \leq n_r^* \leq r(h-1) + n_r$
Number of reactions	$r^* = hr$
Number of linkage classes	$\ell^* \leq \ell$
Rank of Network	$s^* = s$
Reactant rank of the network	$q^* = c$
Rank Difference	$\Delta(\mathscr{N})^* = s - c$
Deficiency of the Network	$\delta \leq \delta^* \leq n + r(h-1) - s - 1$

classses may be reduced. This happens when there exists additional complex that is equal to an original complex or another additional complex. Hence, $\ell^* \leq \ell$ (as shown in Table 3.1). Moreover, the number of terminal linkage class is impossible to decrease after the transformation. With this, $t^* \leq t$ (see Table 3.1).

For the deficiency of the network and reactant rank of the network, we refer to the next section of this paper.

3.3. Invariance of CRN properties under STAR-RVM Transformation

At this point, we explore the different CRN properties that are invariant under the STAR-RVM transformation. We study necessary and/or sufficient conditions that are required for these properties to be invariant under the transformation.

3.3.1. *t-minimality*

We observe from Example 11 that the number of linkage classes ℓ is 1 and the number of terminal strong linkage classes t is also 1. Since $\ell = t$, $\mathscr{N}$ is t-minimal. Note that we have $\ell^* = 1$ and $t^* = 2$ and so $\mathscr{N}^*$ is not t-minimal. This tells us that if $\mathscr{N}$ is t-minimal then $\mathscr{N}^*$ is **not necessarily** t-minimal. With this, we will inject conditions on a t-minimal network in order to have a t-minimal STAR-RVM transform network stated as follows:

Proposition 7. *Let $\mathscr{N}$ be a poly-PL system with a poly-PL kinetics of $h = 2$ and $\mathscr{N}^*$ be the STAR-RVM transform of $\mathscr{N}$. If $\mathscr{N}$ is t-minimal and for every complex y of $\mathscr{N}$, $d^-(y) + d^+(y) = 1$ then $\mathscr{N}^*$ is t-minimal.*

Proof. Let $\mathscr{N}$ be a poly-PL systems with a poly-PL kinetics of $h = 2$ and $\mathscr{N}^*$ be the STAR-RVM transform of $\mathscr{N}$. Suppose $\mathscr{N}$ is t-minimal and for every complex y, $d^-(y) + d^+(y) = 1$.

Since $\mathscr{N}$ is t-minimal, the number of linkage classes l is equal to the number of terminal strong linkage classes t. This assures that no original complex reacts to a complex belonging to a different strong linkage class.

Since for every complex y, $d^-(y) + d^+(y) = 1$, we can partition the set of complexes to pairs where each equivalence class is given by $\{y, y'\}$ such that $y \to y'$.

Constructing $\mathscr{N}^*$, note that since $h = 2$ we will add one complex y^* and reaction $y' \to y^*$ or $y^* \to y$.

Now, if each y^* is not equal to any of the original complexes or any additional complexes then there will be no changes in the number of linkage classes and terminal strong linkage classes. Hence, the equality of l and t still holds. Thus, $\mathscr{N}^*$ is t-minimal.

On the other hand, suppose a particular additional complex $y_1^* \in \{y_2, y_2', y_2^*\}$ of the reactions $y_2 \to y_2' \to y_2^*$ or $y_2^* \to y_2 \to y_2'$. With this, the linkage class where y_1^* belongs and the linkage class of $\{y_2, y_2', y_2^*\}$ will be merged. Hence, the number linkage of classes and terminal strong linkage classes will be both decreased by one. Thus, the equality of l and t still holds and therefore $\mathscr{N}^*$ is t-minimal.

For the next property, we will explore the weakly reversibility of STAR-RVM transform.

3.3.2. *Weakly Reversibility*

Example 12 shows that if $\mathscr{N}$ is weakly reversible, $\mathscr{N}^*$ is **not always** weakly reversible. Notice that the network $\mathscr{N}$ is a cycle. Hence, $\mathscr{N}$ is weakly reversible. With the corresponding STAR-RVM transform, we note that the additional reactions r_1^*, r_2^* and r_3^* do not belong to any cycle. Thus, $\mathscr{N}^*$ is not weakly reversible. Hence, the following states the sufficient condition for a weakly reversible network to have a weakly reversible STAR-RVM transform netwok:

Proposition 8. *If for every reaction $y \to y'$ of a weakly reversible network $\mathscr{N}$ the last additional complex y^* in STAR-RVM transform N^* is equal to any of the original complex of $\mathscr{N}$, then $\mathscr{N}^*$ is weakly reversible.*

Proof. Let $\mathscr{N}$ be a weakly reversible network and $\mathscr{N}^*$ be the STAR-RVM transform of $\mathscr{N}$. Recall that the original complexes are part of the complexes of $\mathscr{N}^*$. Thus, the symmetry property of directed path in the said complexes still holds.

Suppose $y \to y'$ is an arbitrary reaction in $\mathscr{N}$ and y^* is the last additional complex in the said reaction that is equal to any original complex. On the same linkage class, let $\widehat{y}$ be any additional complex in the reaction. If $\widehat{y}$ is an original complex then the symmetry property of directed path (there is directed path from one complex to another and vice versa) holds in this case.

Now, for the case that $\widehat{y}$ is not equal to any original complex. By the construction of STAR-RVM, there is a directed path from y to $\widehat{y}$, $y \Rightarrow \widehat{y}$ (or for the other case of STAR-RVM, $\widehat{y} \Rightarrow y$). We have to show that there exist $\widehat{y} \Rightarrow y$ ($y \Rightarrow \widehat{y}$), respectively.

Since $\widehat{y} \neq y^*$ and by the fact that $\widehat{y}$ and y^* are both additional complexes on the same reaction, there exist $\widehat{y} \Rightarrow y^*$ ($y^* \Rightarrow \widehat{y}$), respectively. And by the fact that y^* is equal to an original complex of a weakly reversible network N, there exists $y^* \Rightarrow y$ ($y \Rightarrow y^*$), respectively. Hence, there exists $\widehat{y} \Rightarrow y$ ($y^* \Rightarrow \widehat{y}$), respectively.

Thus, in $\mathscr{N}^*$, whenever there is $y_a \Rightarrow y_b$ we also have $y_b \Rightarrow y_a$ and so $\mathscr{N}^*$ is weakly reversible.

Similar with weakly reversibility, cycle terminal property is not conserved in the STAR-RVM transform as dicussed in the next section.

3.3.3. *Cycle Terminal Property*

In Example 12, observe that $n = n_r$. This implies that $\mathscr{N}$ is cycle terminal. But after finding the STAR-RVM transform, $n^* = 6 \neq 3 = n_r^*$ indicating that $\mathscr{N}^*$ is not cycle terminal.

Thus, the cycle terminal property is not invariant under the STAR-RVM transformation. Hence, we have the following sufficient condition.

Proposition 9. *If for every reaction $y \to y'$ of a cycle terminal network $\mathscr{N}$ the last additional complex y^* in STAR-RVM transform $\mathscr{N}^*$ is equal to any original complex or additional complex, then $\mathscr{N}^*$ is cycle terminal.*

Proof. Let $\mathscr{N}$ be a cycle terminal network where n is the number of complexes and n_r is the number of reactant complexes. This means that $n = n_r$. Constructing $\mathscr{N}^*$ by STAR-RVM method, let n^* be the number of complexes and n_r^* be the number of reactant complexes of $\mathscr{N}^*$. We have to show that $n^* = n_r^*$

Let x be the number of additional complexes. Suppose that for every reaction $y \to y'$ of $\mathscr{N}$, the last additional complex y^* in $\mathscr{N}^*$ is equal to any original complex or additional complex. This implies that all additional complexes are source vertices. Hence, $n^* = n+x$ and $n_r^* = n_r + x$.

Thus, $n^* - n_r^* = (n + x) - (n_r + x) = n - n_r = 0$. Therefore, $n^* = n_r^*$ and $\mathscr{N}^*$ is cycle terminal.

In the next section, we discuss the first property that is invariant under the STAR-RVM transformation.

3.3.4. *Point Terminal Property*

On the next proposition, we show that the STAR-RVM transform of a point terminal network is also point terminal.

Proposition 10. *If a poly-PL system $(\mathscr{N}, K)$ is point terminal, its STAR-RVM transform $(\mathscr{N}*, K*)$ is also point terminal.*

Proof. Let $(\mathscr{N}, K)$ be a poly-PL systems and $(\mathscr{N}^*, K^*)$ be the its STAR-RVM transform. Suppose $\mathscr{N}$ is point terminal. This means that $t = n - n_r$ where t is the number of terminal strong linkage classes, n is the number of complexes and n_r be the number of reactant complexes.

Let $T = \{\{y\} | y$ is a complex such that $d^+(y) = 0\}$. Hence, $t = |T|$. Constructing $\mathscr{N}^*$ by STAR-RVM method, we let t^* be the number of terminal strong linkage classes, n^* the number of complexes and n_r^* the number of reactant complexes. We have to show $t^* = n^* - n_r^*$. We divide our proof into two parts corresponding to the cases defined on of STAR-RVM.

Case 1 (for case (i) in STAR-RVM):
Let $T^* = \{\{y^*\} | y^*$ is an additional complex such that $d^+(y^*) = 0\}$. Observe that $t^* = |T^*|$ since , by the construction, t^* is the number of additional complexes that serves as target only vertices.

Let x be the number of additional complex y'^* such that $d^+(y'^*) \neq 0$. This implies that the number of additional complexes is $x + t^*$ and $n^* = n + x + t^*$. Also, observe that by the definition of STAR-RVM transform, $n_r^* = n_r + t + x$.

Now,

$$\begin{aligned} n^* - n_r^* &= (n + x + t^*) - (n_r + t + x) \\ &= n + x + t^* - n_r - t - x) \\ &= [(n - n_r) - t] + t^* \\ &= t^*. \end{aligned}$$

Case 2 (for case (ii) in STAR-RVM):
Note that if each additional complex is not equal to any element of T, we have $t^* = n^* - n_r^*$ in STAR-RVM transform.

Suppose there exists an additional complex that is equal to an element of T. Let y be the number additional complexes in this case that is equal to any element of T and z is the number of other additional complexes. This implies that $n^* = n + z$, $n_r^* = n_r + z + y$ and $t^* = t - y$.

Now,

$$\begin{aligned} n^* - n_r^* &= (n + z) - (n_r + z + y) \\ &= n - n_r - y \\ &= [(n - n_r) - t] + t - y \\ &= t^*. \end{aligned}$$

3.3.5. *Equality of Rank*

We show that the dimension of the stoichiometric subspace of the original network and its STAR-RVM transform are equal.

Proposition 11. *If* $(\mathscr{N}, K)$ *is a poly-PL system and* $(\mathscr{N}^*, K^*)$ *its STAR-RVM transform then* $s = s^*$.

Proof. Recall that $S = span\{y' - y \in \mathbb{R}^{\mathscr{S}} : y \to y' \in \mathscr{R}\}$ is the stoichiometric subspace of $\mathscr{N}$ and $s = dim\ \ S$. Observe that for a reaction $y \to y'$ in $\mathscr{N}$, each reaction or complex in $\mathscr{N}^*$ by STAR-RVM method is in the form:

$$y \to y' \to y' + (y' - y) \to y' + 2(y' - y) \to \dots \quad or$$

$$\dots \to y + 2(y - y') \to y + (y - y') \to y \to y'$$

With this, a reaction vector of $\mathscr{N}^*$ is in the form $y' - y$. This implies that the stoichiometric subspace of $\mathscr{N}^*$ is $S^* = span\{y' - y \in \mathbb{R}^{\mathscr{S}} : y \to y' \in \mathscr{R}\}$. Hence, $S^* = S$ and $s^* = s$.

3.3.6. *Terminality Bounded by Deficiency (TBD) and Sufficient Reactant Deficiency (SRD)*

Another two properties conserved under STAR-RVM method are the TBD and SRD as discussed in the next propositions and corollaries.

Proposition 12. *Let* $(\mathscr{N}, K)$ *be a poly-PL system and* $(\mathscr{N}^*, K^*)$ *be its STAR-RVM transform. If* $\mathscr{N}$ *is of TBD type so is* $\mathscr{N}^*$.

Proof. Let $(\mathscr{N}, K)$ be a poly-PL systems and $(\mathscr{N}^*, K^*)$ be its STAR-RVM transform. Suppose $\mathscr{N}$ is of TBD type. This means that

$$t - \ell \leq \delta = n - \ell - s.$$

Hence,

$$t \leq n - s.$$

With this, we have to show that

$$t^* \leq n^* - s^*.$$

We present the proof in two parts.

i. Suppose $t^* \leq t$.

Recall that, $n \leq n^*$ and $s = s^*$. This implies that $n - s \leq n^* - s^*$. Hence

$$t^* \leq t \leq n - s \leq n^* - s^*.$$

ii. Suppose $t^* > t$.

This means that $n^* > n$ and $(t^* - t), (n^* - n) \in Z^+$.

By the construction of N^* using STAR-RVM method, observe that $t^* - t = |\{\{y^*\} : y^*$ is an additional complex such that $d^+(y^*) = 0\}|$ and $n^* - n$ is the number of additional complexes not equal to any original or other additional complex. Note that, by the fact that y^* is an additional complex such that $d^+(y^*) = 0$, all such v^*'s are unique. Hence,

$$t^* - t \leq n^* - n.$$

Thus,

$$\begin{array}{rcl} t & \leq & n - s \\ t + (t^* - t) & \leq & n - s + (n^* - n) \\ t^* & \leq & n^* - s \\ t^* & \leq & n^* - s^*. \end{array}$$

Therefore,

$$t^* - \ell^* \leq n^* - \ell^* - s^* = \delta^*$$

implying that $\mathscr{N}^*$ is also of TBD type.

We recall that a TBD network is SRD. This means that SRD property should also be conserved after the method. This was reflected on the following proposition.

Proposition 13. *Let $(\mathscr{N}, K)$ be a poly-PL system and $(\mathscr{N}^*, K^*)$ be its STAR-RVM transform. If $\mathscr{N}$ has sufficient reactant diversity (SRD) then $\mathscr{N}^*$ has also sufficient reactant diversity (SRD).*

Proof. Let $\mathscr{N}$ be a poly-PL system and $\mathscr{N}^*$ be the STAR-RVM transform of $\mathscr{N}$. Suppose $\mathscr{N}$ has SRD. This means that $n_r \geq s$.

Recall that, $n_r^* \geq n_r$ and $s^* = s$.

Thus,

$$n_r^* \geq n_r \geq s = s^*.$$

Therefore ,N^* has also SRD).

Corollary 2. *: Let N be a poly-PL systems with a poly-PL kinetics of $h = 2$ and N^* be the STAR-RVM transform of $\mathscr{N}$. If $\mathscr{N}$ is t-minimal and for every complex v, $d^-(v) + d^+(v) = 1$ then N^* is SRD network*

3.3.7. *Complex Factorizability*

One of the most important kinetic properties is complex factorizability. To explore the said property with regards to STAR-RVM method, we consider the following example.

Example 13. *For* $(\mathscr{N}, K)$*, suppose* $\mathscr{S} = \{X, Y\}$ *and* $\mathscr{R} = \{r :_1 X + Y \to X + 2Y, r_2 : X + 2Y \to 2X + 2Y$*. Let the poly-PL kinetics be given by:*

$$K_{r1}(X, Y) = k_2(X^2Y + XY^2)$$

$$K_{r2}(X, Y) = k_3(X + X^2Y^2)$$

where k_1 *and* k_2 *are rate constants.*

Note that the given $(\mathscr{N}, K)$ *is complex factorizable* $(PLK - RDK)$*. Generating STAR-RVM transform, we have* $(\mathscr{N}^*, K^*)$ *where* $\mathscr{S} = \{X, Y\}$ *and* $\mathscr{R}^* = \{r_1 : X + Y \to X + 2Y, r_1^* = X + 2Y \to X + 3Y, r_2 : X + 2Y \to 2X + 2Y, r_2^* : 2X + 2Y \to 3X + 2Y\}$*. The kinetic functions are as follows:*

$$K^*_{r1}(X, Y) = k^*_2 X^2Y$$

$$K^*_{r1^*}(X, Y) = k^{**}_2 XY^2$$

$$K^*_{r2}(X, Y) = k^*_3 X$$

$$K^*_{r2^*}(X, Y) = k^{**}_3 X^2Y^2.$$

Observe that the kinetic order of the reactant $X + 2Y$ *for the reactions* r_1^* *and* r_2 *are not equal. Thus,* $(\mathscr{N}^*, K^*)$ *is not* $PLK - RDK$ *and so is not complex factorizable.*

With this, we have the following proposition stating conditions that assure complex factorizability of $\mathscr{N}^*$ given that $\mathscr{N}$ is.

Proposition 14. *Let* $(\mathscr{N}, K)$ *be a poly-PL system of* $h = 2$ *and* $(\mathscr{N}^*, K^*)$ *be the STAR-RVM transform. If* $(\mathscr{N}, K)$ *is complex factorizable satisfying the following:*

i. for every complex y*, either* $d^-(y) = 0$ *or* $d^+(y) = 0$ *(but not both),*

ii. the components of the reaction vectors in N *are all positive or equal to zero*

then $(\mathscr{N}^*, K^*)$ *is complex factorizable.*

Proof. Let $(\mathscr{N}, K)$ be a poly-PL kinetic system with a poly-PL kinetics of $h = 2$ and $(\mathscr{N}^*, K^*)$ be the STAR-RVM transform.

Since $(\mathscr{N}, K)$ is complex factorizable, it is $PLK - RDK$. This implies that if there are reactions with the same reactant complexes, they have equal kinetic orders. Also, since the components of the reaction vectors in $\mathscr{N}$ are all nonnegative then only case (i) of STAR-RVM applies.

Now, take note of the following on STAR-RVM transform $(\mathscr{N}^*, K^*)$:

(a) Since for every complex y, either $d^{-}(y) = 0$ or $d^{+}(y) = 0$ (but not both), then a complex is either a reactant complex or a product complex. This assures us that the reactant complexes on additional reactions on N^* are original product complexes which are different from the original reactant complexes.

(b) Since $h = 2$, we are sure that the additional complexes on the additional reactions are all product complexes.

By (a) and (b), the state where the reactions with the same reactant complexes, have equal kinetic order was maintained. Hence, $(\mathscr{N}^*, K^*)$ is $PLK - RDK$ and complex factorizable.

In the next section, we identify the bounds on $\mathscr{N}^*$ of one important property of CRN which is the deficiency of the network δ^*.

3.3.8. *Deficiency of the network*

By the construction of STAR-RVM, the number of complexes is most likely increased but the number of linkage classes is most likely decreased. These cases are important to consider on how the deficiency of the network in STAR-RVM transform changes.

In the next proposition, we present the bounds for the said property:

Proposition 15. *Let $(\mathscr{N}, K)$ be a poly-PL system and $(\mathscr{N}^*, K^*)$ be the STAR-RVM transform. Given the deficiency δ of the network N, then the deficiency δ^* of the network $\mathscr{N}^*$, is given by*

$$\delta \leq \delta^* \leq n + r(m-1) - s - 1.$$

where n is the number of complexes, ℓ is the number of linkage classes and s is the dimension of the stoichiometric subspace of the network $\mathscr{N}$.

Proof. Observe that:

i. $n \leq n^*$ because of the possible additional complexes

ii. $\ell^* \leq \ell$ since STAR-RVM method does not produce additional linkage class but rather it can lessen the number of original linkage classes which happens when there exist additional complexes which are equal to some original complexes.

With the two observations, we can say that

$$n - \ell \leq n^* - \ell^*. \tag{3}$$

Recall that from Proposition 11, that $s^* = s$.

By (3),

$$\begin{aligned} n - \ell - s &\leq n^* - \ell^* - s^* \\ \delta &\leq \delta^*. \end{aligned}$$

Given the number of terms in K, h and number of reactions r in $\mathscr{N}$, it can be observed that the maximum number of additional complexes in $\mathscr{N}^*$ is $(h-1)r$.

Thus,

$$\delta \leq \delta^* \leq n + r(h-1) - \ell^* - s.$$

Since $\ell \geq 1$,

$$\delta \leq \delta^* \leq n + r(h-1) - s - 1.$$

3.3.9. *Reactant Rank*

The following proposition tells about the effect of the STAR-RVM transformation on the reactant rank of the network.

Proposition 16. *Let $(\mathscr{N}, K)$ be a poly-PL system and $(\mathscr{N}^*, K^*)$ be the STAR-RVM transform. The reactant rank of $\mathscr{N}^*$ is $q^* = c$, where c is the rank of the linear subspace generated by the all the complexes.*

Proof. Let $(\mathscr{N}, K)$ be a poly-PL systems and $(\mathscr{N}^*, K^*)$ be the STAR-RVM transform. Also, let q^* be the reactant rank of N^*.

Note that for a reaction $y \to y'$ in $\mathscr{N}$, the reactions and complexes in $\mathscr{N}^*$ by STAR-RVM method is in the form:

$$y \to y' \to y' + (y' - y) \to y' + 2(y' - y) \to \dots$$

or

$$y + (h-1)(y - y') \to \cdots \to y + 2(y - y') \to y + (y - y') \to y \to y'$$

Observe that all additional reactant complexes from every reaction $y \to y'$ in this transformed network are linear combinations of y and y'. This implies that all reactant complexes of $\mathscr{N}^*$ are linear combinations of the complexes in $\mathscr{N}$. Hence, the reactant rank $q^* = c$.

4. Conclusion

STAR transformations from PYK to PLK is introduced leading to analyses of power law kinetics and their invariant properties. The transformation is defined by constructing CRN using additional complexes and reactions using multiple reaction vectors. A comparison of the network numbers of the original network and its transformed network lead us to the identification variant and invariant properties brought about by these transformations.

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