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Mathematical Formulation of Stoichiometric Subspaces Associated with Chemical Reaction Networks: The Linear Algebraic Foundations and Fundamentals

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Abstract:- The article presents a consolidated review of the mathematical framework for construction of Stoichiometric subspaces associated with Chemical Reaction Networks, based on theoretically imposed constraints, mechanistic considerations and data driven mathematical modeling; A rigorous mathematical treatment of the problem is presented and is illustrated using an appropriate numerical case study example.

Keywords:- *Stoichiometric Matrix, Chemical Reaction Networks, Fundamental Subspaces of a Matrix, Stoichiometric Subspaces, Chemical Factor Analysis.*

➢ ***Notations***

- R^n denotes the Real co-ordinate space of dimension ' n '
- $\hat{M}_{x\times y}(R)$ denotes the Real Matrix space of order ' x ' by ' y '
- $A_{x\times y}$, $B_{x\times y}$ be real valued matrices; $A_{x\times y} \geq B_{x\times y}$ implies that $a_{ij} \geq b_{ij}$ for every $(i, j)^{th}$ slot , where $i = 1, 2, ..., x; j = 1, 2, ..., y$
- $(A_{x\times y})^T$ denotes the transpose of the matrix $A_{x\times y}$
- $I_{w\times w}$ denotes the Identity Matrix of order ' w '
- W , V be subspaces of R^n ; $V \subseteq W$ implies that the vector space V is a proper or an improper subspace of the vector space W
- $\dim.[V]$ denotes the dimension of the vector space V
- $A_{x\times y} \in \hat{M}_{x\times y}(R)$; $Csp(A_{x\times y})$ denotes the Column space of the matrix $A_{x\times y}$ and $Nsp(A_{x\times y})$ denotes the Null space of the matrix $A_{x\times y}$
- 'SVD' is the abbreviation of 'Singular Value Decomposition'
- $diag(y_1, y_2, ..., y_w)$ denotes a diagonal matrix of order ' w ' whose diagonal entries along the main diagonal, from top to bottom, are $y_1, y_2, ..., y_w$ respectively.

I. INTRODUCTION

A Chemical Reaction Network involves a set of chemical species interlinked among each other through one or more chemical reaction transformations [4,8,10], the dynamical behavior of such reaction networks can be quite intricate but governed in general to a significant extent, by the stoichiometric relationships that exists among these chemical species that constitute the network. It is therefore of great importance, to have a systematic mathematical framework to express and to analyze the stoichiometric interrelationship structure associated with a reaction network problem; these type of problems are an integral component in the domains such as chemical reaction engineering or mathematical modeling of metabolic networks in biological systems [1,2,3,4,5,8, 9,10,11].

The Stoichiometric matrix [1,2,3,5,8,9,10,11] is a mathematical construct that provides a coherent mathematical representation of the stoichiometric structure associated with a reaction network, the remarkable utility of this mathematical form stems from the underlying linear algebraic implications; the vector subspaces associated with a stoichiometric matrix (the four fundamental subspaces associated with the stoichiometric matrix [7,12]) provide various useful information about the associated chemical reaction network, for example, the dynamic and the steady state components of the flux vector and mass conservation constraint conditions [8].

The present article attempts to provide a comprehensive review of the different types of Stoichiometric subspaces that can be formulated for chemical reaction networks under the consideration of several types of chemical constraints to be satisfied by reaction stoichiometric vectors; in this regard, the article attempts to consolidate upon the ideas presented in the previous research studies [1,2,3,10,11] and construct a consolidated treatment and an associated rigorous mathematical framework. In the present discussion, the Theoretical Stoichiometric subspace is formulated by taking

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into consideration the Atomic and Charge conservation constraints to be satisfied by every feasible reaction stoichiometric vector associated with the reaction network whereas the Mechanistic Stoichiometric subspace is generated explicitly from the stoichiometric matrix associated with the chemical reaction network under consideration. It is to be noted that every experimental measurement of observable properties related to reaction networks would invariably be associated with experimental error and thus attempting to solve Blind Matrix equations to estimate Stoichiometric matrix from experimental Data matrix would in general, over estimate the true size of the underlying Latent space (Factor Space) [3,6]. The mathematical framework of Chemical Factor Analysis and Target testing [3,6] to validate postulated reaction stoichiometries, can help to estimate the true size of the Factor space generating the data and to estimate the Stoichiometric subspace associated with the reaction network producing the data; this estimated Stoichiometric subspace is commonly referred to as the Observed Stoichiometric subspace. The article presents a numerical case study based on a hypothetical chemical reaction network to illustrate the computation of the associated Theoretical, Mechanistic and the Observed, Stoichiometric subspaces.

The article is an attempt to provide an exposure of the linear algebraic foundations and fundamentals of the Stoichiometric matrices and their extreme utility in dealing with problems related to unraveling the properties of chemical reaction networks, thereby attempting to bring the topic of reaction stoichiometries and their associated vector subspaces, closer to the mainstay of traditional chemistry curricula.

II. PROPERTIES OF CHEMICAL REACTION NETWORKS

A Chemical Reaction Network (abbreviated as C.R.N) is formally designated as:

- $\Omega(m, n, p \mid x1, x2, ..., xm \mid A_1, A_2, ..., A_n \mid E_1, E_2, ..., E_p)$,

➢ *Formulation of the Associated Stoichiometric Matrix* $S_{m\times n}$ *:*

$$S_{m\times n} = \begin{bmatrix} \nu_{11} & \nu_{12} & . & . & \nu_{1n} \\ \nu_{21} & \nu_{22} & . & . & \nu_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ \nu_{m1} & \nu_{m2} & . & . & \nu_{mn} \end{bmatrix},$$

Where we have the following:

- $m =$ Number of Chemical reactions constituting the C.R.N
- $n =$ Number of Chemical species constituting the C.R.N
- $p =$ Number of Chemical elements constituting the C.R.N
- $\lambda =$ Cardinality of the maximum sized Linearly Independent set of Chemical reactions possible for the given C.R.N
- Constituent chemical species: $A_1, A_2, ..., A_n$
- Constituent chemical elements: $E_1, E_2, ..., E_p$
- Constituent chemical reactions: $x1, x2, ..., xm$

➢ *The Chemical Reaction Network Framework*

$x1: \nu_{11}A_1 + \nu_{12}A_2 + ... + \nu_{1n}A_n = 0$,

$x2: \nu_{21}A_1 + \nu_{22}A_2 + ... + \nu_{2n}A_n = 0$

upto $xm: \nu_{m1}A_1 + \nu_{m2}A_2 + ... + \nu_{mn}A_n = 0$

$\nu_{ij} =$ Stoichiometric coefficient associated with the chemical species A_j for the chemical reaction xi ,

Where $i = 1, 2, ..., m;\ j = 1, 2, ..., n$

- $\nu_{ij} > 0$ if the species A_j participates as product in the chemical reaction xi
- $\nu_{ij} < 0$ if the species A_j participates as reactant in the chemical reaction xi
- $\nu_{ij} = 0$ if the species A_j does not participate in the chemical reaction xi

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We define:

$$\psi(i)_{n\times 1} = \begin{bmatrix} \nu_{i1} \\ \nu_{i2} \\ . \\ . \\ \nu_{in} \end{bmatrix}$$

Where $i = 1, 2, ..., m$

$\psi(i)_{n\times 1} =$ Stoichiometric vector associated with the chemical reaction xi

$(S_{m\times n})^T = [\psi(1)_{n\times 1} \quad \psi(2)_{n\times 1} \quad . \quad . \quad \psi(m)_{n\times 1}]$,

We have the following:

- $\dim.[Csp((S_{m\times n})^T)] = \text{rank}\,[S_{m\times n}] = \lambda$, $Csp((S_{m\times n})^T) \subseteq R^n$
- $Csp((S_{m\times n})^T)$ is termed as the " Mechanistic Stoichiometric Subspace " associated with the C.R.N

➢ *Formulation of the Associated Atomic Matrix* $G_{p\times n}$ *:*

- $\theta_{ab} =$ number of atoms of chemical element E_a in the chemical species A_b , where $a = 1, 2, ..., p; b = 1, 2, ..., n$

$$G_{p\times n} = \begin{bmatrix} \theta_{11} & \theta_{12} & . & . & \theta_{1n} \\ \theta_{21} & \theta_{22} & . & . & \theta_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ \theta_{p1} & \theta_{p2} & . & . & \theta_{pn} \end{bmatrix},$$

Therefore $G_{p\times n} \geq 0_{p\times n}$

➢ *Formulation of the Associated Charge Quanta Matrix* $M_{1\times n}$ *:*

- $q_j =$ Quanta of electronic charge associated with the chemical species A_j , where $j = 1, 2, ..., n$
- $q_j > 0$ for the positively charged species A_j , $q_j < 0$ for the negatively charged species A_j and $q_j = 0$ for the uncharged species A_j
- $q_j \in \{0, \pm 1, \pm 2, ...\} \quad \forall j = 1, 2, ..., n$
- $M_{1\times n} = [q_1 \quad q_2 \quad . \quad . \quad q_n]$

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➢ *Formulation of the Constraint Matrix* $J_{(p+1)\times n}$ *:*

$$J_{(p+1)\times n} = \begin{bmatrix} G_{p\times n} \\ M_{1\times n} \end{bmatrix} = \begin{bmatrix} \theta_{11} & \theta_{12} & . & . & \theta_{1n} \\ \theta_{21} & \theta_{22} & . & . & \theta_{2n} \\ . & . & . & . & . \\ . & . & . & . & . \\ \theta_{p1} & \theta_{p2} & . & . & \theta_{pn} \\ q_1 & q_2 & . & . & q_n \end{bmatrix},$$

$$\dim.[Nsp(J_{(p+1)\times n})] = \delta$$

- $Nsp(J_{(p+1)\times n})$ is termed as the " Theoretical Stoichiometric Subspace " associated with the C.R.N , where $Nsp(J_{(p+1)\times n}) \subseteq R^n$.

➢ *The Principle of Atomic and Charge Conservation in a Chemical Reaction Network:*

- Any constituent reaction xi where $i = 1,2,....,m$, of the C.R.N , satisfies the following set of equality constraints:

✓ $\theta_{11}\nu_{i1} + \theta_{12}\nu_{i2} + ... + \theta_{1n}\nu_{in} = 0$, $\theta_{21}\nu_{i1} + \theta_{22}\nu_{i2} + ... + \theta_{2n}\nu_{in} = 0$ upto

✓ $\theta_{p1}\nu_{i1} + \theta_{p2}\nu_{i2} + ... + \theta_{pn}\nu_{in} = 0$

✓ Therefore, $G_{p\times n}\psi(i)_{n\times 1} = 0_{p\times 1} \quad \forall i = 1,2,....,m$ this implies that: $G_{p\times n}(S_{m\times n})^T = 0_{p\times m}$

✓ We also have $q_1\nu_{i1} + q_2\nu_{i2} + ... + q_n\nu_{in} = 0 \quad \forall i = 1,2,....,m$, therefore $M_{1\times n}\psi(i)_{n\times 1} = 0 \quad \forall i = 1,2,....,m$, this implies $M_{1\times n}(S_{m\times n})^T = 0_{1\times m}$

- $G_{p\times n}(S_{m\times n})^T = 0_{p\times m}$: The principle of Atomic Conservation in the C.R,N
- $M_{1\times n}(S_{m\times n})^T = 0_{1\times m}$: The principle of Charge Conservation in the C.R.N.

Therefore $J_{(p+1)\times n}(S_{m\times n})^T = 0_{(p+1)\times m}$, hence we have $Csp((S_{m\times n})^T) \subseteq Nsp(J_{(p+1)\times n})$ which implies $\lambda \le \delta$

➢ *The Framework of Observed Stoichiometric Subspace Associated with a Chemical Reaction Network*

- $y_j =$ A measurable property associated with the constituent chemical species A_j , where $j = 1,2,....,n$
- $\omega_i =$ An intrinsic property associated with the constituent chemical reaction xi , where $i = 1,2,....,m$

We assume the following form of linear interrelationships:

- $y_1 = \omega_1\nu_{11} + \omega_2\nu_{21} + ... + \omega_m\nu_{m1}$, $y_2 = \omega_1\nu_{12} + \omega_2\nu_{22} + ... + \omega_m\nu_{m2}$ upto
- $y_n = \omega_1\nu_{1n} + \omega_2\nu_{2n} + ... + \omega_m\nu_{mn}$
- $c =$ Number of independent observations on the set of variables: $y_1, y_2, ..., y_n$

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Therefore, we generate the following Matrix equation:

- $Y_{c\times n} = Z_{c\times m} S_{m\times n}$ (eqn.1)

Where we have:

$$Y_{c\times n} = \begin{bmatrix} y_1(1) & y_2(1) & . & . & y_n(1) \\ y_1(2) & y_2(2) & . & . & y_n(2) \\ . & . & . & . & . \\ . & . & . & . & . \\ y_1(c) & y_2(c) & . & . & y_n(c) \end{bmatrix},$$

$$Z_{c\times m} = \begin{bmatrix} \omega_1(1) & \omega_2(1) & . & . & \omega_m(1) \\ \omega_1(2) & \omega_2(2) & . & . & \omega_m(2) \\ . & . & . & . & . \\ . & . & . & . & . \\ \omega_1(c) & \omega_2(c) & . & . & \omega_m(c) \end{bmatrix}$$

$y_j(t) =$ Value of the property y_j for the t^{th} observation, $\omega_i(t) =$ Value of the property ω_i for the t^{th} observation, where $t = 1, 2, ..., c$ $\hat{Y}_{c\times n}$: The experimentally measured Data matrix $\mathrm{H}_{c\times n}$: The Experimental error Matrix, therefore we have: $\hat{Y}_{c\times n} = Y_{c\times n} + \mathrm{H}_{c\times n} = Z_{c\times m} S_{m\times n} + \mathrm{H}_{c\times n}$ (eqn 2)

rank($\hat{Y}_{c\times n}$) = f, since the experimental error manifests in general as contributions across all available degrees of freedom or across those degrees of freedom not contributing to the pure data, we have: $\lambda \le f$

SVD of $\hat{Y}_{c\times n}$: $\hat{Y}_{c\times n} = U_{c\times f} \Sigma_{f\times f} (V_{n\times f})^T$, where we have the following:

- $U_{c\times f} = \begin{bmatrix} U(1)_{c\times\lambda} & U(2)_{c\times(f-\lambda)} \end{bmatrix}$, $(U_{c\times f})^T U_{c\times f} = I_{f\times f}$
- $V_{n\times f} = \begin{bmatrix} V(1)_{n\times\lambda} & V(2)_{n\times(f-\lambda)} \end{bmatrix}$, $(V_{n\times f})^T V_{n\times f} = I_{f\times f}$
- $\Sigma_{f\times f} = \begin{bmatrix} \Sigma(1)_{\lambda\times\lambda} & 0_{\lambda\times(f-\lambda)} \\ 0_{(f-\lambda)\times\lambda} & \Sigma(2)_{(f-\lambda)\times(f-\lambda)} \end{bmatrix}$, $\Sigma(1)_{\lambda\times\lambda} = diag(\sigma_1, \sigma_2, ..., \sigma_\lambda)$,
- $\Sigma(2)_{(f-\lambda)\times(f-\lambda)} = diag(\sigma_{\lambda+1}, \sigma_{\lambda+2}, ..., \sigma_f)$ Where $\sigma_1 \ge \sigma_2 \ge .... \ge \sigma_\lambda \ge \sigma_{\lambda+1} \ge \sigma_{\lambda+2} \ge .... \ge \sigma_f > 0$
- $\bar{Y}_{c\times n}$: rank= λ approximation to the matrix $\hat{Y}_{c\times n}$, $\bar{Y}_{c\times n} = U(1)_{c\times\lambda} \Sigma(1)_{\lambda\times\lambda} (V(1)_{n\times\lambda})^T$ (eqn.3)
- $Csp(V(1)_{n\times\lambda}) \subseteq R^n$, $Csp(V(1)_{n\times\lambda})$ is termed as the " *Observed Stoichiometric Subspace* " associated with the C.R.N , $\dim.[Csp(V(1)_{n\times\lambda})] = \mathrm{rank}(\bar{Y}_{c\times n}) = \lambda$

➢ *Efficiency of Alignment of the Subspaces:*

- $P_{n\times n} = V(1)_{n\times\lambda} (V(1)_{n\times\lambda})^T$, $P_{n\times n}$ is the Orthogonal Projector onto $Csp(V(1)_{n\times\lambda})$
- $B_{n\times\lambda} = \begin{bmatrix} b(1)_{n\times1} & b(2)_{n\times1} & . & . & b(\lambda)_{n\times1} \end{bmatrix}$,
- $B_{n\times\lambda}$ is an Orthonormal basis matrix of $Csp((S_{m\times n})^T)$, therefore we have the following:
- $(B_{n\times\lambda})^T B_{n\times\lambda} = I_{\lambda\times\lambda}$, $Q_{n\times n} = B_{n\times\lambda} (B_{n\times\lambda})^T$ is the Orthogonal Projector onto $Csp((S_{m\times n})^T)$

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We define: $\eta(\%) = [(\frac{1}{\lambda})\sum_{r=1}^{\lambda}(b(r)_{n\times 1})^T(V(1)_{n\times\lambda}(V(1)_{n\times\lambda})^T)b(r)_{n\times 1}]\times 100$ (eqn.4)

$\eta(\%)$ is defined as the "*Percentage Alignment efficiency*" of $Csp((S_{m\times n})^T)$ with respect to $Csp(V(1)_{n\times\lambda})$; it is therefore a quantitative estimate of the overlap of the Mechanistic and the Observed, Stoichiometric subspaces.

- $\eta(\%) = [(\frac{1}{\lambda})trace[P_{n\times n}Q_{n\times n}]]\times 100 = [(\frac{1}{\lambda})trace[Q_{n\times n}P_{n\times n}]]\times 100$ (eqn.5)

➢ *Numerical Case Study*

In this section, a hypothetical Chemical reaction network is formulated and analyzed to illustrate the mathematical framework presented in the previous section.

$x1: CO_3^{-2} + H^+ \leftrightarrow HCO_3^- \; x2: HCO_3^- + H^+ \leftrightarrow H_2O + CO_2 \; x3: OH^- + H^+ \leftrightarrow H_2O \; x4: HCO_3^- + OH^- \leftrightarrow H_2O + CO_3^{-2}$

Therefore, we have the following set of associated results:

- Constituent Chemical Elements: $E_1 = C, E_2 = O, E_3 = H$
- Constituent Chemical Species:
- $A_1 = CO_3^{-2}, A_2 = H^+, A_3 = HCO_3^-, A_4 = H_2O, A_5 = CO_2, A_6 = OH^-$
- $m = 4, n = 6, p = 3$
- $q_1 = -2$, $q_2 = 1$, $q_3 = -1$, $q_4 = q_5 = 0$ and $q_6 = -1$

Atomic Matrix

$$G_{3\times 6} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 3 & 0 & 3 & 1 & 2 & 1 \\ 0 & 1 & 1 & 2 & 0 & 1 \end{bmatrix},$$

Charge Quanta Matrix

$$M_{1\times 6} = \begin{bmatrix} -2 & 1 & -1 & 0 & 0 & -1 \end{bmatrix},$$

Therefore we have

Constraint Matrix

$$J_{4\times 6} = \begin{bmatrix} 1 & 0 & 1 & 0 & 1 & 0 \\ 3 & 0 & 3 & 1 & 2 & 1 \\ 0 & 1 & 1 & 2 & 0 & 1 \\ -2 & 1 & -1 & 0 & 0 & -1 \end{bmatrix}, \quad \dim.[Nsp(J_{4\times 6})] = \delta = 3$$

Stoichiometric Matrix $S_{4\times 6} = \begin{bmatrix} -1 & -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 1 & 0 & -1 \end{bmatrix}$, $\dim.[Csp((S_{4\times 6})^T)] = \lambda = 3$

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In the case of the particular C.R.N under consideration, we have $Nsp(J_{4\times6}) = Csp((S_{4\times6})^T) = \Gamma$, $\Gamma \subseteq R^6$, $\Gamma = \{w_{6\times1} \in R^6 \mid w_{6\times1} = B_{6\times3}\alpha_{3\times1}, \alpha_{3\times1} \in R^3\}$ where we have:

$$B_{6\times3} = \begin{bmatrix} 1 & 0 & 4 \\ 1 & 0 & -2 \\ -1 & 0 & 2 \\ 0 & 1 & -3 \\ 0 & 0 & -6 \\ 0 & -1 & -3 \end{bmatrix}_{6\times3} \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{78}} \end{bmatrix}_{3\times3}, \quad \alpha_{3\times1} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$$

where $\alpha_1, \alpha_2, \alpha_3 \in R$

$B_{6\times3}$ is an Orthonormal Basis matrix for the Subspace Γ

We choose $c = 8$ and the following hypothetical linear framework in formulating the Observed Stoichiometric subspace $\overline{\Gamma}$:

$$\hat{U}_{8\times3} = (\frac{1}{\sqrt{8}}) \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & -1 \\ 1 & -1 & -1 \\ 1 & -1 & 1 \end{bmatrix}, \quad \hat{\Sigma}_{3\times3} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad H_{8\times6} = (0.1) \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}_{8\times1} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}_{1\times6}$$

$\hat{Y}_{8\times6} = \hat{U}_{8\times3}\hat{\Sigma}_{3\times3}(B_{6\times3})^T + H_{8\times6}$, $\overline{Y}_{8\times6}$ is the rank=3 approximation of the matrix $\hat{Y}_{8\times6}$ based on SVD of $\hat{Y}_{8\times6}$ and reconstruction using contribution only from the first three leading singular values and the corresponding modes (the associated pair of 1 dimensional Row and Column subspaces)

$\overline{Y}_{8\times6} = U(1)_{8\times3}\Sigma(1)_{3\times3}(V(1)_{6\times3})^T$ Where we have:

$$U(1)_{8\times3} = \begin{bmatrix} -0.331091 & 0.353553 & 0.374672 \\ -0.374672 & 0.353553 & -0.331091 \\ -0.374672 & 0.353553 & -0.331091 \\ -0.331091 & 0.353553 & 0.374672 \\ -0.331091 & -0.353553 & 0.374672 \\ -0.374672 & -0.353553 & -0.331091 \\ -0.374672 & -0.353553 & -0.331091 \\ -0.331091 & -0.353553 & 0.374672 \end{bmatrix}, \quad \Sigma(1)_{3\times3} = \begin{bmatrix} 2.269145 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0.992058 \end{bmatrix},$$

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$$V(1)_{6\times3} = \begin{bmatrix} -0.620011 & 0 & 0.544979 \\ -0.638464 & 0 & -0.138524 \\ 0.389643 & 0 & 0.173669 \\ -0.133637 & 0.707107 & -0.324179 \\ -0.142863 & 0 & -0.665931 \\ -0.133637 & -0.707107 & -0.324179 \end{bmatrix}$$

$$Csp(V(1)_{6\times3}) = \bar{\Gamma}\ ,\ \bar{\Gamma} \subseteq R^6\ ,\ \bar{\Gamma} = \{\bar{w}_{6\times1} \in R^6 \mid \bar{w}_{6\times1} = V(1)_{6\times3}\alpha_{3\times1}, \alpha_{3\times1} \in R^3\}\ ,$$

Therefore we have: η (%) = 97.45 %

III. CONCLUDING REMARKS

The chemical reaction networks associated with real world problems are in general comprising of enormous number of constituent reactions and involve a very large number of constituent chemical species, therefore the associated Stoichiometric matrices are very large sized but they do possess intricate interrelationships among the matrix elements, dimensionality reduction techniques based on SVD can be utilized to reduce large matrices to a suitable lower rank approximation which would capture the requisite variation in data but would require much lesser storage space[7,12].

In most realistic situations, the set of chemical reactions that constitute a Multicomponent reaction system is not completely known, so an accurate mechanistic construction of the stoichiometric matrix is impossible in this situation; here data driven, factor analytical studies [3,6] provides an approach to obtain an estimate, however, in a general situation, it is not always possible to measure the entire set of response variables that encompass every chemical species constituting the network, the situation where not all constituent chemical species are measured and a factor analytical study is utilized to identify the plausible stoichiometric models, is discussed in [3].

The constraints imposed through the chemical requirements of atomic and charge conservation impose restriction which lead to postulation of a lower dimensional subspace of the co-ordinate space, as the plausible vector space that encompasses the true stoichiometric subspace, in real world situations, the dimensionality intrinsic to the problem is very large and so these set of constraints, although can be quite large in number, may still be inadequate to reasonably reduce the dimensionality in terms of the postulated stoichiometric space. In the study of metabolic pathway analysis [5, 8, 9], the constraints are imposed on feasible reaction stoichiometries by invoking requirements of elemental, charge and moiety balance.

The mathematical modeling of chemical reaction networks, both in domains of pure chemistry or in biology, leads to a lot of useful information but presents several challenges as well. The Stoichiometric matrix is a ubiquitous component of every such reaction network; however, to adequately understand the dynamical behavior of such networks, it is essential to analyze the properties of the system of non-linear differential equations generated from such a reaction network. A consolidated, authoritative discussion on chemical reaction network theory is presented in [4]. It is of utmost hope and extreme importance that a serious study of the theory and applications of chemical reaction networks be incorporated at the core of academic curricula associated with chemistry education, at one or more academic levels.

REFERENCES

[1]. Aris, R., and Mah, R.H.S., Independence of chemical reactions, Ind. Engng Chem. Fundam. Vol 2, pp. 90-94 (1963)
[2]. Bjòrnbom, P.H., The independent reactions in calculations of complex chemical equilibria, Ind. Engng Chem. Fundam. Vol 14, pp. 102-106 (1975)
[3]. Bonvin, D., and Rippin, D.W.T., Target Factor Analysis for the Identification of Stoichiometric Models, Chemical Engineering Science, Vol 45, No. 12, pp. 3417-3426 (1990)
[4]. Feinberg, Martin, Foundations of Chemical Reaction Network Theory, Springer Maarleveld, Timo R., Khandelwal, Ruchir A., Olivier, Brett G., Teusink, Bas, Bruggeman, Frank J., Basic concepts and principles of Stoichiometric modeling of metabolic networks, Biotechnology Journal, Vol 8(9), pp. 997-1008 (2013)
[5]. Malinowski, Edmund. R., Factor Analysis in Chemistry, Third Edition, John Wiley and Sons Inc.
[6]. Meyer, Carl. D., Matrix Analysis and Applied Linear Algebra, SIAM
[7]. Nakhleh, Luay, Bioinformatics: Network Analysis-Analyzing Stoichiometric Matrices (Lecture Slides, Department of Computer Science, Rice University) (2013)

ISSN No:-2456-2165 https://doi.org/10.38124/ijisrt/IJISRT24MAY964

[8]. Palsson, Bernhard, Representing Reconstructed Networks Mathematically: The Stoichiometric Matrix (Lecture Slides, Department of Bioengineering, University of California, San Diego) (2003)
[9]. Rawlings, James. B., Stoichiometry of Chemical Reactions, (Lecture notes, Department of Chemical and Biological Engineering, University of Wisconsin-Madison) (2014)
[10]. Rawlings, J. B., and Ekerdt, J. G., Chemical Reactor Analysis and Design Fundamentals, Second Edition, Nob Hill Publishing Strang, Gilbert, Linear Algebra and its Applications, Fourth Edition, Cengage Learning.