

## 화학반응식 균형과 안정성을 위한 새로운 유사 역행렬법

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### A New Pseudoinverse Matrix Method For Balancing Chemical Equations And Their Stability

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⊙Balancing the equation of the reaction is a matter of mathematics only.⊙  
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**요약.** 이 논문에 화학반응식 균형을 맞추기 위한 새로운 유사 역행렬법이 기술되었다. 여기에 제공된 방법은 Moore-Penrose 유사 역행렬을 사용한 Diophantine 행렬식의 해에 기초를 둔다. 방법은 전형적인 여러 화학반응식에 시험 적용되었고 폭넓은 균형연구에서 모든 반응식에 매우 성공적이었다. 이 방법은 아무 제한없이 성공적으로 적용되고, 또한 새로운 화학반응식의 타당성에 대한 검증력도 있고, 만일 새식이 타당하다면 화학식 균형을 이룰 것이다. 여기서 다루어진 화학반응식들은 소수산화수를 지닌 원자를 포함하고 있다. 또한, 화학반응식의 확장된 행렬의 안정성에 대한 화학반응식의 안정성의 필요충분조건을 이 연구에 소개하였다.

**주제어:** 유사 역행렬, 화학반응식 균형 맞추기, 안정성

**ABSTRACT.** In this work is given a new pseudoinverse matrix method for balancing chemical equations. Here offered method is founded on virtue of the solution of a Diophantine matrix equation by using of a Moore-Penrose pseudoinverse matrix. The method has been tested on several typical chemical equations and found to be very successful for the all equations in our extensive balancing research. This method, which works successfully without any limitations, also has the capability to determine the feasibility of a new chemical reaction, and if it is feasible, then it will balance the equation. Chemical equations treated here possess atoms with fractional oxidation numbers. Also, in the present work are introduced necessary and sufficient criteria for stability of chemical equations over stability of their extended matrices.

**Keywords:** Pseudoinverse Matrix, Balancing Chemical Equations, Stability

## 1. INTRODUCTION

Chemical equations are the most exploited part of theoretical as well as industrial chemistry. Every chemistry instructor doubtless has his favorite technique of balancing equations. Chemical equations are commonly written for two purposes: to show the probable reaction products, and to show the

quantities of materials that enter into reaction. It is fortunate indeed that an extensive and comprehensive knowledge of sub-atomic phenomena is not essential in the balancing of equations. Every student, which has general chemistry as an obligatory subject, is bound to come across balancing chemical equations. It is highly important for chemistry student to be able to write and balance chemical

equations readily and accurately. Actually, balancing chemical equations provides an excellent demonstrative and pedagogical example of interconnection between stoichiometrical principles and linear algebra.

A *chemical equation* is a symbolic representation of a *chemical reaction*. The substances initially involved in a chemical reaction are called *reactants*, but the newly formed substances are called the *products*. The products are new substances with properties that are different from those of reactants. Classically, chemical reactions encompass changes that strictly involve the motion of *electrons* in the forming and breaking of *chemical bonds*, although the general concept of a chemical reaction, in particular the notion of a *chemical equation*, is applicable to *transformations of elementary particles*.

A chemical equation is not only the shorthand writing of the chemist, but it should be a mental picture of an actual reaction. To the observant investigator, the equation should immediately remind him as to the physical nature and properties of the reactants, *viz.*, color, state, etc., as well as the chemical result and its physical nature. Thus, a great deal of significance should be attached to the writing of chemical equations. The part of chemical mathematics called *Stoichiometry* deals with the weight relations determined by chemical equations and formulas. According to it, the balancing of chemical equations is important in this area. Since a chemical reaction, when it is feasible, is a natural process, the consequent equation is always consistent. Therefore, we must have a nontrivial solution and we should be able to obtain it assuming its existence. Such an assumption is absolutely valid and does not introduce any error. If the reaction is infeasible, then the only solution is a trivial one, *i. e.*, the all coefficients are equal to zero.

## 2. HISTORICAL SURVEY

During the past years, numerous articles have appeared in scientific literature relative to the balancing of chemical equations. In this section is made a short survey of selected articles for balanc-

ing chemical equations. The selection criteria for references were intentionally wide, in order to include a large variety of topics. Balancing chemical equations in the scientific literature is considered from four points of view: mathematical, computational, chemical and pedagogical.

Now, shortly we will describe these glances.

Jones for the first time in mathematics proposed the general problem for balancing chemical equations.<sup>1</sup> Krishnamurthy in his article<sup>2</sup> gave an algebraic approach for balancing chemical equations founded on virtue of a generalized matrix inverse. Little bit late Das<sup>3</sup> offered a simple scholarly technique, which was discussed in.<sup>4,5</sup> One other technique for balancing chemical equation over an integer programming approach is given in,<sup>6</sup> while in<sup>7</sup> by using of a reflexive generalized inverse matrix is solved the general problem of balancing chemical equations given in.<sup>1</sup> The newest mathematical results for balancing chemical equations and their stability over a nonsingular matrix method are obtained in.<sup>8</sup> Actually, to date in mathematics and chemistry there are only three strictly formalized consistent mathematical methods for balancing chemical equations, particularly they are the methods given in<sup>7,8</sup> and right now presented method in this work, while other so called *methods* in chemical sense have a limited usage, and they are useful only for particular cases, especially for balancing chemical equations which possess atoms with integer oxidation numbers.

In chemistry there are many published articles,<sup>9-29</sup> which consider the use of computers for balancing chemical equations. All of these computational methods use some commercial softer packet.

University textbooks of general chemistry generally support the ion-electron technique as basic procedure for balancing chemical equation, because it makes the best use of fundamental chemical principles. Also, some authors advocated other techniques, which involve less algebraic manipulation that may deserve attention - particularly in classes of chemistry and chemical engineering majors.<sup>30-56</sup>

Several simple chemical equations are solved by elementary algebraic techniques in.<sup>4,5,57-62</sup> Bottom-

ley published the earliest article that makes use of the linear algebra method.<sup>63</sup> A set of various modifications, which implement this approach, is documented in.<sup>31,44,45,64-66</sup> The case when the chemical equation has no unique solution received considerable attention in the education articles.<sup>18,67-79</sup> The equation represents two or more independently occurring reactions can be combined in varying stoichiometric ratios.<sup>80,81</sup> Fixed ratios of reagents, observed experimentally in particular cases, are equivalent to a restriction on the coefficients that make a unique solution.<sup>18</sup>

It is necessary to stress out that balancing chemical equations by inspection is equivalent to using the algebraic method or a computerized matrix algebra approach.<sup>82,83</sup> The valence change method<sup>80,84-106</sup> and the ion-electron method<sup>85-88,92,100,107-113</sup> are also simple algebraic inspection techniques, subjected to exactly the same controls and limitations as the algebraic and matrix methods. Here it is good to emphasize that first Karslake in<sup>114</sup> considered balancing of ionic chemical equations. Actually, the technique suggested by Garcia<sup>115</sup> can reduce the number of algebraic steps for ion-electron method. Above both mentioned methods - the valence change method and ion-electron method begin by establishing the relative proportions of reagents taking part in separate oxidation and reduction components of a redox reaction. Then, each technique uses a lowest common multiplier to enforce a principle of conservancy - for instance, conservation of oxidation number change in the case of the oxidation number method. Johnson in his article<sup>116</sup> defined the equivalent term *oxidation stage change* on this subject.

Stout in<sup>117</sup> presented three redox reactions as puzzles. Each one can be shown as simple redox system, which may easily be balanced using here offered method. After this article was published, the followed other debatable articles with critical accent.<sup>118-123</sup>

Balancing chemical equations through the pedagogical point of view is given in the articles.<sup>112,124-133</sup> This approach is very interesting for the education of chemical research. A check of the hypothesis

that formal reasoning and a sufficiently large mental capacity are required to balance more complex many-step equations is made over a test to determine level of intellectual development, mental capacity, and degree of field dependence/field independence of the students.<sup>134</sup>

### 3. PRELIMINARIES

Now we will introduce some well known results from the matrix algebra. Throughout, the set of  $m \times n$  matrices over a field will be denoted by  $\mathbb{R}^{m \times n}$ .

**Definition 3. 1.** *The Moore-Penrose pseudoinverse  $A^-$  of a matrix  $A \in \mathbb{R}^{m \times n}$  is the unique matrix satisfying the following criteria:  $AA^-A = A$ ,  $A^+AA^- = A^+$ ,  $(AA^-)^T = AA^+$ ,  $(A^+A)^T = A^+A$ .*

Suppose the matrix  $A$  has full rank, then

$$A = [a_{ij}]_{n \times n} \text{ and } \text{rank } A = n \Rightarrow A^- = A^{-1},$$

$$A = [a_{ij}]_{m \times n} \text{ (} m > n \text{) and } \text{rank } A = n \Rightarrow A^- = (A^T A)^{-1} A^T,$$

$$A = [a_{ij}]_{m \times n} \text{ (} m < n \text{) and } \text{rank } A = m \Rightarrow A^+ = A^T (A A^T)^{-1}.$$

If the matrix  $A$  does not have full rank, i.e.,  $A$  is an  $m \times n$  matrix and  $\text{rank } A = r < \min(m, n)$ , then pseudoinverse  $A^+$  can be constructed from the singular value decomposition  $A = UDV^T$  by  $A^- = VD^+U^T$ .

Also the Moore-Penrose pseudoinverse  $A^+$  of a matrix  $A$ , we can derive on this way. There do always exist two matrices  $C = [c_{ij}]_{m \times r}$  and  $D = [d_{ij}]_{r \times n}$  of rank  $r$ , such that  $A = CD$ . Using these matrices it holds that  $A^- = D^+(DD^+)^{-1}(C^T C)^{-1}C^T$ .

Pseudoinverse matrix  $A^-$  of a matrix  $A$  was independently defined by Moore<sup>135</sup> and Penrose<sup>136</sup>. If the matrix  $A^-$  satisfies first two equalities of definition 3. 1, then it is called a *reflexive generalized inverse* of  $A$ , denoted by  $A^-$ . This matrix is not unique.

**Definition 3. 2.** *The characteristic equation of an  $n \times n$  matrix  $A$  is the equation in one variable  $\lambda$*

$$\det(A - \lambda I) = 0 \tag{3.1}$$

where  $\det(\cdot)$  denotes a determinant and  $I$  is an  $n \times n$  identity matrix.

**Definition 3. 3.** *The polynomial*

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \dots + a_1 \lambda + a_0 = 0 \tag{3.2}$$

which results from evaluating the determinant (3.1)

is the characteristic polynomial of the matrix  $A$ .

The above polynomial of degree  $n \geq 1$  with real coefficients  $a_i$  ( $0 \leq i \leq n$ ), where  $a_n \neq 0$ , by the fundamental theorem of algebra has  $n$  (not necessarily distinct) roots  $\lambda_1, \lambda_2, \dots, \lambda_n$ .

**Definition 3. 4.** The roots of the characteristic polynomial (3. 2) are precisely the eigenvalues of the matrix  $A$ .

**Definition 3. 5.** The reaction matrix has the following format  $A|B = [A|B]_{m \times (r+s)}$ , where  $A = [a_{ij}]_{m \times r}$  ( $r < m$ ) and  $B = [b_{ij}]_{m \times s}$  ( $s < m$ ).

**Definition 3. 6.** An extended matrix

$$\text{Ext}A|B = \begin{bmatrix} A & B \\ \mathbf{O} & I \end{bmatrix} \quad (3.3)$$

of  $(r+s) \times (r+s)$  dimension, is singular if  $\det(\text{Ext}A|B) = 0$ , where  $A = [a_{ij}]_{m \times r}$  ( $r < m$ ),  $B = [b_{ij}]_{m \times s}$  ( $s < m$ ),  $I$  is the identity matrix of  $(r+s-m) \times (r+s-m)$  dimension and  $\mathbf{O}$  is a zero matrix of  $(r+s-m) \times m$  dimension.

In<sup>8</sup> is treated the non-singular case.

Let  $\sigma(\text{Ext}A|B) = \{\lambda_i, 1 \leq i \leq k\}$  be the spectrum of  $\text{Ext}A|B$ . Let  $|\cdot|$  denotes a vector norm in  $\mathbb{R}^n$ .

**Definition 3. 7.** The Lozinskii measure  $\mu$  on  $\mathbb{R}^n$  with respect to  $|\cdot|$  is defined by

$$\mu(\text{Ext}A|B) = \lim_{\rho \rightarrow 0} (|\mathbf{I} + \rho \text{Ext}A|B| - 1) / \rho. \quad (3.4)$$

**Definition 3. 8.** The Lozinskii measures of  $\text{Ext}A|B = [a_{ij}]_{r \times r}$  with respect to the three common norms

$$\begin{aligned} |x|_1 &= \sup_j |x_j|, \\ |x|_2 &= \sum_j |x_j|, \\ |x|_2 &= (\sum_j |x_j|^2)^{1/2}, \end{aligned} \quad (3.5)$$

are

$$\begin{aligned} \mu_1(\text{Ext}A|B) &= \sup_k (a_{kk} + \sum_{k \neq i} |a_{ik}|), \\ \mu_2(\text{Ext}A|B) &= \sup_k (a_{kk} + \sum_{i \neq k} |a_{ik}|), \\ \mu_2(\text{Ext}A|B) &= \text{stab}\{[(\text{Ext}A|B) + (\text{Ext}A|B)^T] / 2\}, \end{aligned} \quad (3.6)$$

where

$$\text{stab}(\text{Ext}A|B) = \max\{\lambda, \lambda \in \sigma(\text{Ext}A|B)\}$$

is the stability modulus of  $\text{Ext}A|B$  and  $T$  denoting transpose.

**Definition 3. 9.** The extended matrix  $\text{Ext}A|B$  is stable if  $\text{stab}(\text{Ext}A|B) < 0$ .

## 4. MAIN RESULTS

In this section we will give a completely new method for balancing and stability of chemical equations. Given analysis is done for arbitrary chemical equation presented in its general form.

**Proposition 4. 1.** Any chemical equation may be presented in this form

$$\sum_{j=1}^r x_j \prod_{i=1}^m \Psi_{ai}^{a_{ij}} = \sum_{j=1}^s y_j \prod_{i=1}^m \Omega_{bi}^{b_{ij}} \quad (4.1)$$

where  $x_j$  ( $1 \leq j \leq r$ ) and  $y_j$  ( $1 \leq j \leq s$ ) are unknown rational coefficients,  $\Psi^i$  and  $\Omega^i$  ( $1 \leq i \leq m$ ) are chemical elements in reactants and products, respectively;  $a_{ij}$  ( $1 \leq i \leq m$ ;  $1 \leq j \leq r$ ) and  $b_{ij}$  ( $1 \leq i \leq m$ ;  $1 \leq j \leq s$ ) are numbers of atoms of elements  $\Psi^i$  and  $\Omega^i$ , respectively, in  $j$ -th molecule.

*Proof.* Let there exists an arbitrary chemical equation from  $s$  distinct elements and  $m+n$  molecules

$$\sum_{j=1}^r x_j \Xi_j = \sum_{j=1}^s y_j \Theta_j \quad (4.2)$$

where  $\Xi_j = \Psi_{a_1}^{a_{1j}} \Psi_{a_2}^{a_{2j}} \dots \Psi_{a_m}^{a_{mj}}$  ( $1 \leq j \leq r$ ) and  $\Theta_j = \Omega_{b_1}^{b_{1j}} \Omega_{b_2}^{b_{2j}} \dots \Omega_{b_m}^{b_{mj}}$  ( $1 \leq j \leq s$ ). Then previous expression becomes

$$\sum_{j=1}^r x_j \Psi_{a_1}^{a_{1j}} \Psi_{a_2}^{a_{2j}} \dots \Psi_{a_m}^{a_{mj}} = \sum_{j=1}^s y_j \Omega_{b_1}^{b_{1j}} \Omega_{b_2}^{b_{2j}} \dots \Omega_{b_m}^{b_{mj}} \quad (4.3)$$

Now, if we write the above equation in a compact form, then immediately follows (4.1).

The coefficients  $x_j, y_j$  satisfy three basic principles (corresponding to a closed input-output static model<sup>137,138</sup>)

- the law of conservation of atoms,
- the law of conservation of mass, and
- the time-independence of the reaction.

**Theorem 4. 2.** The chemical equation (4.1) can be reduced to the following Diophantine matrix equation

$$Ax = By, \quad (4.4)$$

where  $A = [a_{ij}]_{m \times r}$  is a matrix of the reactants,  $B = [b_{ij}]_{m \times s}$  is a matrix of the products,  $x^T = (x_1, x_2, \dots, x_r)$

and  $y^T=(y_1, y_2, \dots, y_r)$  are column vectors of unknown coefficients and  $T$  denotes transpose.

*Proof.* If we develop the molecules of the reaction (4.1) in an explicit form, then we obtain a matrix of the reactants  $A$

$$A = \begin{matrix} \Psi^1_{a11} \Psi^2_{a12} \dots \Psi^m_{a1m} & \Psi^1_{a21} \Psi^2_{a22} \dots \Psi^m_{a2m} & \dots & \Psi^1_{a_{r1}} \Psi^2_{a_{r2}} \dots \Psi^m_{a_{rm}} & \Psi^1 \\ & a_{21} & & a_{2r} & \Psi^2 \\ & a_{31} & & a_{3r} & \Psi^3 \\ & & & & \dots \\ & & & & \Psi^m \end{matrix}$$

and a matrix of the products  $B$

$$B = \begin{matrix} \Omega^1_{b11} \Omega^2_{b12} \dots \Omega^s_{b1s} & \Omega^1_{b21} \Omega^2_{b22} \dots \Omega^s_{b2s} & \dots & \Omega^1_{b_{r1}} \Omega^2_{b_{r2}} \dots \Omega^s_{b_{rs}} & \Omega^1 \\ & b_{21} & & b_{2s} & \Omega^2 \\ & b_{31} & & b_{3s} & \Omega^3 \\ & & & & \dots \\ & & & & \Omega^s \end{matrix}$$

From the above development we obtain that

$$\Xi_j = \sum_{i=1}^m a_{ij} \Psi^i \quad (1 \leq j \leq r) \quad (4.5)$$

and

$$\Theta_j = \sum_{i=1}^m b_{ij} \Omega^i \quad (1 \leq j \leq s) \quad (4.6)$$

If we substitute (4.5) and (4.6) into (4.2), follows

$$\sum_{j=1}^r x_j \sum_{i=1}^m a_{ij} \Psi^i = \sum_{j=1}^s y_j \sum_{i=1}^m b_{ij} \Psi^i \quad (4.7)$$

or

$$\sum_{i=1}^m \Psi^i \sum_{j=1}^r a_{ij} x_j = \sum_{i=1}^m \Omega^i \sum_{j=1}^s b_{ij} y_j \quad (4.8)$$

i.e., the above expression holds if only if

$$\sum_{j=1}^r a_{ij} x_j = \sum_{j=1}^s b_{ij} y_j \quad (1 \leq i \leq m) \quad (4.9)$$

Last equation if we present in a matrix form, actually we obtain (4.4).

Now we will prove the following result.

**Theorem 4.3.** Let  $A \in \mathbb{R}^{m \times r}$  and  $B \in \mathbb{R}^{m \times s}$ . The matrix Diophantine equation (4.4) is consistent if and only if for some  $A^-$

$$Gy = 0, \quad (4.10)$$

where

$$G = (I - AA^+)B. \quad (4.11)$$

If this is the case, a representation of the general solution is

$$y = (I - G^-G)u \quad (4.12)$$

and

$$x = A^-By + (I - A^-A)v, \quad (4.13)$$

with arbitrary vectors  $u \in \mathbb{R}^{r-1}$  and  $v \in \mathbb{R}^{r-1}$ .

*Proof.* Matrix equation (4.4) is consistent if and only if there exist vectors  $x \in \mathbb{R}^{r-1}$  and  $y \in \mathbb{R}^{s-1}$  such that

$$Ax - By = 0. \quad (4.14)$$

From (4.13) we have  $Ax = AA^-By$ , since  $A(I - A^-A) = 0$ . Thus, from (4.14) follows

$$Ax - By = AA^-By - By = -(I - AA^+)By = -Gy; \text{ since (4.11).} \quad (4.15)$$

On the other hand, from (4.12) it follows that

$$Gy = G(I - G^-G)u = 0, \text{ since } G = GG^-G. \quad (4.16)$$

Immediately, from (4.16) and (4.15) follows (4.4).

**Remark 4.4.** This theorem generalizes the theorem proved in [1]. By the above theorem, a century old chemistry problem of balancing chemical equations in a general form is completely solved.

**Definition 4.5.** Chemical equation (4.1) is stable if  $\text{stab}(\text{Ext}A|B) < 0$ .

**Lemma 4.6.** For any nonsingular matrix  $U$  and any vector norm  $|\cdot|$ , with the induced Lozinskiĭ measure  $\mu$ ,  $|Ux|$  defines another vector norm and its induced matrix measure  $\mu_U$  is given by

$$\mu_U(\text{Ext}A|B) = \mu[U(\text{Ext}A|B)U^{-1}]. \quad (4.17)$$

*Proof.* The proof of this lemma follows directly from the definition 3.7.

**Theorem 4.7.** For any matrix  $\text{Ext}A|B \in \mathbb{R}^n$  it holds

$$\text{stab}(\text{Ext}A|B) = \inf\{\mu(\text{Ext}A|B), \mu \text{ is a Lozinskiĭ measure on } \mathbb{R}^n\}. \quad (4.18)$$

*Proof.* The relation (4.18) obviously holds for diagonalizable matrices in view of (4.17) and the first two relations in (3.6). Furthermore, the infimum in (4.18) can be achieved if the matrix  $\text{Ext}A|B$  is diagonalizable. The general case can be shown based on this observation, the fact that  $\text{Ext}A|B$  can be

approximated by diagonalizable matrices in and the continuity of  $\mu(\cdot)$ , which is implied by the property

$$|\mu(\mathcal{J}) - \mu(\mathcal{N})| \leq |\mathcal{J} - \mathcal{N}|.$$

**Remark 4. 8.** From the above proof it follows that

$$\text{stab}(\text{Ext}A|B) = \inf\{\mu_{\cdot}[U(\text{Ext}A|B)U^{-1}], \det U \neq 0\}.$$

The same relation holds if  $\mu$  is replaced by  $\mu_1$ .

**Corollary 4. 9.** Let  $\text{Ext}A|B \in \mathbb{R}$ . Then  $\text{stab}(\text{Ext}A|B) < 0 \Leftrightarrow \mu(\text{Ext}A|B) < 0$  for some Lozinskii measure  $\mu$  on  $\mathbb{R}^n$ .

There are more results for stability criteria obtained in the works.<sup>139,140</sup>

For the matrices  $A$  and  $B$  given in the theorem 4.2, let  $\text{rank}A|B = \rho$  and  $\text{ker}A|B = \kappa$ , where  $\text{ker}$  denotes the nullity or kernel of matrix  $A|B$ . According to<sup>141</sup>, the deterministic approach is important, since it enables us to classify the chemical reaction as:

1° *infeasible* when the nullity of the reaction matrix  $A|B$  is zero;

2° *unique* (within relative proportions) when the nullity of the reaction matrix  $A|B$  is one; or

3° *non-unique* when the nullity of the reaction matrix  $A|B$  is bigger than one.

Possible cases of balancing chemical equations are the following

1. If  $m \geq r + s = \rho$ , then  $\kappa = r + s - \rho = 0$ , i. e., trivial solution  $x, y = 0$ , the reaction is infeasible.

2. If  $m \geq r + s, \rho = r + s - 1$ , then  $\kappa = r + s - \rho = 1$ , unique solution  $x, y > 0$ , i. e., the reaction is feasible and is unique.

In practical terms this means that the general procedure for obtaining these coefficients is to solve the system of linear equations derived from the principles of conservation of matter and charge, applied to the reaction element-by-element.

3. If  $m \geq r + s, \rho < r + s - 1$ , then  $\kappa = r + s - \rho > 1$ ,  $\kappa (> 1)$  linearly independent solutions  $x, y > 0$ , i. e., the reaction is feasible and is non-unique.

4. If  $m < r + s, \rho \leq m$ , then  $\kappa = r + s - \rho \geq 1$ ,  $\kappa (\geq 1)$  linearly independent solutions  $x, y > 0$ , i. e., the reaction is feasible and is non-unique.

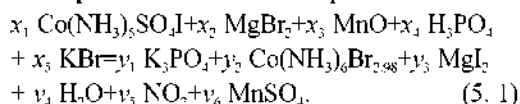
Last two kinds of the reactions are puzzling in that they exhibit infinite linearly independent solution all of which satisfy the chemical balance, and yet they are not all chemically feasible solutions for a given set of experimental conditions. A unique solution is obtained by imposing a chemical constraint, namely, that reactants have to react only in certain proportions.

## 5. AN APPLICATION OF THE MAIN RESULTS

In this section will be applied above method on many chemical equations for their balancing. All chemical equations balanced here appear first time in professional literature and they are chosen with an intention to be avoided to date all well know chemical equations which were repeated many times in the chemical journals for explanation of certain particular techniques for balancing of some chemical equations using only atoms with integer oxidation numbers.

1° First we will consider an infeasible reaction, i. e., the case when the nullity of the reaction matrix is zero.

**Example 5. 1.** Consider this equation



By the schemes

	$\text{Co}(\text{NH}_3)_5\text{SO}_4$	$\text{MgBr}_2$	$\text{MnO}$	$\text{H}_3\text{PO}_4$	$\text{KBr}$	$\text{K}_3\text{PO}_4$	$\text{Co}(\text{NH}_3)_6\text{Br}_2$	$\text{MgI}_2$	$\text{H}_2\text{O}$	$\text{NO}_2$	$\text{MnSO}_4$		
<b>A</b>	1	0	0	0	0	0	1	0	0	0	0	Co	
	5	0	0	0	0	0	6	0	0	1	0	N	
	15	0	0	3	0	0	18	0	2	0	0	H	
	1	0	0	0	0	0	0	0	0	0	1	S	
	4	0	1	4	0	4	0	0	1	2	4	O	
	1	0	0	0	0	0	0	2	0	0	0	I	
	0	1	0	0	0	0	0	1	0	0	0	Mg	
	0	2	0	0	1	0	2.98	0	0	0	0	0	Br
	0	0	1	0	0	0	0	0	0	0	1	0	Mn
	0	0	0	1	0	1	0	0	0	0	0	0	P
	0	0	0	0	1	3	0	0	0	0	0	0	K

are determined the matrix of reactants  $A$  and the matrix of the products  $B$ , an according to it the

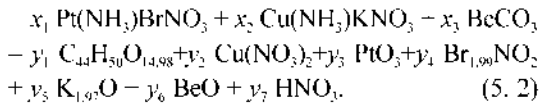
reaction matrix  $A|B$  obtains the form

$$A|B = \begin{bmatrix} 1.00 & 0 & 0 & 0 & 0 & 0 & 1.00 & 0 & 0 & 0 & 0 \\ 5.00 & 0 & 0 & 0 & 0 & 0 & 6.00 & 0 & 0 & 1 & 0 \\ 15.0 & 0 & 0 & 3 & 0 & 0 & 18.0 & 0 & 2 & 0 & 0 \\ 1.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 0 & 0 & 0 & 1 \\ 4.00 & 0 & 1 & 4 & 0 & 4 & 0.00 & 0 & 1 & 2 & 4 \\ 1.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 2 & 0 & 0 & 0 \\ 0.00 & 1 & 0 & 0 & 0 & 0 & 0.00 & 1 & 0 & 0 & 0 \\ 0.00 & 2 & 0 & 0 & 1 & 0 & 2.98 & 0 & 0 & 0 & 0 \\ 0.00 & 0 & 1 & 0 & 0 & 0 & 0.00 & 0 & 0 & 0 & 1 \\ 0.00 & 0 & 0 & 1 & 0 & 1 & 0.00 & 0 & 0 & 0 & 0 \\ 0.00 & 0 & 0 & 0 & 1 & 3 & 0.00 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The rank of the above matrix is  $\rho = 11$ . Since the nullity of the reaction matrix is  $\kappa = r + s - \rho = 5 + 6 - 11 = 0$ , then we have only a trivial solution  $x, y = 0$ , that means that the reaction is infeasible.

2° Next, we will consider the case when the chemical reaction is feasible and is unique, *i. e.*, the nullity of its reaction matrix is one. Here we will balance many special chemical equations with a goal to show the power of the offered mathematical method.

**Example 5. 2.** As a next example to illustrate above method, we will balance this chemical equation



From the schemes given below

	Pt(NH <sub>3</sub> )BrNO <sub>3</sub>		Cu(NH <sub>3</sub> )KNO <sub>3</sub>		Cu(NO <sub>3</sub> ) <sub>2</sub>		PtO <sub>3</sub>		Br <sub>1.99</sub> NO <sub>2</sub>		K <sub>1.97</sub> O		BeO		HNO <sub>3</sub>		
<b>A</b>	1	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	Pt
	2	2	0	0	0	2	0	1	0	0	0	0	0	1	0	0	N
	3	3	0	50	0	0	0	0	0	0	0	0	0	1	0	0	H
	1	0	0	0	0	0	0	1.99	0	0	0	0	0	0	0	0	Br
	3	3	3						2	1	1	3					O
	0	1	0						0	1	0	0	0	0	0	0	Cu
	0	1	0						0	0	0	1.97	0	0	0	0	K
	0	0	1						0	0	0	0	1	0	0	0	Be
	0	0	1	44	0	0	0	0	0	0	0	0	0	0	0	0	C

are determined the matrix of reactants  $A$  and the matrix of the products  $B$ , *i. e.*,

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 2 & 0 \\ 3 & 3 & 0 \\ 1 & 0 & 0 \\ 3 & 3 & 3 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \text{ and } B = \begin{bmatrix} 0.000 & 0 & 1 & 0.00 & 0.00 & 0 & 0 \\ 0.000 & 2 & 0 & 1.00 & 0.00 & 0 & 1 \\ 50.00 & 0 & 0 & 0.00 & 0.00 & 0 & 1 \\ 0.000 & 0 & 0 & 1.99 & 0.00 & 0 & 0 \\ 14.98 & 6 & 3 & 2.00 & 1.00 & 1 & 3 \\ 0.000 & 1 & 0 & 0.00 & 0.00 & 0 & 0 \\ 0.000 & 0 & 0 & 0.00 & 1.97 & 0 & 0 \\ 0.000 & 0 & 0 & 0.00 & 0.00 & 1 & 0 \\ 44.00 & 0 & 0 & 0.00 & 0.00 & 0 & 0 \end{bmatrix}$$

The reaction matrix  $A|B$ , according to the definition 3. 5 obtains the form

$$A|B = \begin{bmatrix} 1 & 0 & 0 & 0.000 & 0 & 1 & 0.00 & 0.00 & 0 & 0 \\ 2 & 2 & 0 & 0.000 & 2 & 0 & 1.00 & 0.00 & 0 & 1 \\ 3 & 3 & 0 & 50.00 & 0 & 0 & 0.00 & 0.00 & 0 & 1 \\ 1 & 0 & 0 & 0.000 & 0 & 0 & 1.99 & 0.00 & 0 & 0 \\ 3 & 3 & 3 & 14.98 & 6 & 3 & 2.00 & 1.00 & 1 & 3 \\ 0 & 1 & 0 & 0.000 & 1 & 0 & 0.00 & 0.00 & 0 & 0 \\ 0 & 1 & 0 & 0.000 & 0 & 0 & 0.00 & 1.97 & 0 & 0 \\ 0 & 0 & 1 & 0.000 & 0 & 0 & 0.00 & 0.00 & 1 & 0 \\ 0 & 0 & 1 & 44.00 & 0 & 0 & 0.00 & 0.00 & 0 & 0 \end{bmatrix}$$

The rank of the above matrix is  $\rho = 9$ . Since the nullity of the reaction matrix is  $\kappa = r + s - \rho = 3 + 7 - 9 = 1$ , then we have only a unique solution, that means that the reaction is feasible. Next, we will determine the solution  $x, y$ .

The Moore-Penrose pseudoinverse  $A^+ = (A^t A)^{-1} A^t$  of the matrix  $A$  is

$$688 A^+ = \begin{bmatrix} 183 & 44 & 66 & 183 & 12 & -161 & -161 & -18 & -18 \\ -161 & 44 & 66 & -161 & 12 & 183 & 183 & -18 & -18 \\ -18 & -72 & -108 & -18 & 168 & -18 & -18 & 92 & 92 \end{bmatrix}$$

and the matrix  $G$  has this form

$$688 G = (688 I - AA^+) B = \begin{bmatrix} -2687.76 & 1.00 & 469.00 & -432.17 & 305.17 & 6.00 & -146.00 \\ -10751.04 & 692.00 & -188.00 & 328.44 & -134.68 & 24.00 & 104.00 \\ 18273.44 & -1026.00 & -282.00 & -539.34 & -202.02 & 36.00 & -188.00 \\ -2687.76 & 1.00 & -219.00 & 936.95 & 305.17 & 6.00 & -146.00 \\ -9314.44 & 564.00 & 324.00 & 152.12 & 88.36 & -56.00 & 216.00 \\ -2687.76 & 345.00 & 125.00 & 252.39 & -372.51 & 6.00 & -146.00 \\ -2687.76 & -343.00 & 125.00 & 252.39 & 982.85 & 6.00 & -146.00 \\ -1164.64 & -846.00 & -486.00 & -228.18 & -132.54 & 428.00 & -324.00 \\ 29107.36 & -846.00 & -486.00 & -228.18 & -132.54 & -260.00 & -324.00 \end{bmatrix}$$

Required vectors  $y$  and  $x$ , according to (4.12) and (4.13) are





nullity of the reaction matrix is  $\kappa - r + s - \rho = 5 + 6 - 10 = 1$ , then we have only a unique solution, that means that the reaction is feasible. Next, we will determine the solution  $x, y$ .

The Moore-Penrose pseudoinverse  $A^+ = (A^T A)^{-1} A^T$  of the matrix  $A$  is

3821829615  $A^+ =$

$$\begin{bmatrix} 530923221 & 661977522 & 654140313 & 530923221 & -175464270 \\ 7914996 & 123779502 & -48555612 & 7914996 & -39240720 \\ -18772587 & -45218394 & 29117439 & -18772587 & 13543215 \\ -271169424 & -152766738 & -354633372 & -271169424 & 637257480 \\ 70185708 & -86901384 & -60307176 & 70185708 & 71450960 \\ \\ 55404972 & -683523900 & -271169424 & 140371416 & 70185708 \\ 51402897 & 68554350 & -12114684 & 31392576 & 15696288 \\ -10122084 & 49154760 & 9177498 & -10834572 & -5417286 \\ -84802788 & 185745600 & 303818211 & -509805984 & -254902992 \\ 109874016 & 44172600 & -254902992 & 1471571078 & 735785539 \end{bmatrix}$$

and the matrix  $G$  has this form

3821829615  $G = (3821829615 I - AA^T)B =$

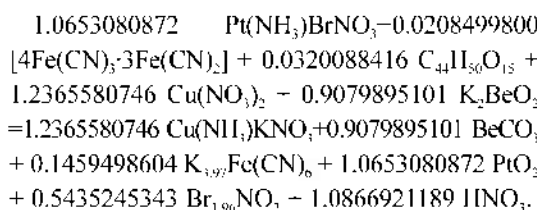
$$\begin{bmatrix} -2629185165.00 & 1139731002.00 & -483401225.52 \\ 1650524550.00 & -803280696.00 & 1845272340.96 \\ 1783528350.00 & -799162944.00 & 25653265.44 \\ -2629185165.00 & 1139731002.00 & -483401225.52 \\ -1131087940.00 & 574862740.00 & -933567342.40 \\ -24135300.00 & 234300654.00 & -5488412135.04 \\ -1641138600.00 & 712163775.00 & 289110156.00 \\ 3485478540.00 & -1842615048.00 & 1910859372.48 \\ 1669236275.00 & -1988622038.00 & 3781386588.23 \\ -1076296670.00 & 2827518596.00 & -5695638491.66 \\ \\ 3641834934.00 & -1351658495.16 & -789725025.00 \\ -1096484442.00 & -1156605852.12 & 198603765.00 \\ -955676193.00 & -1308663759.48 & 226220040.00 \\ -179994681.00 & 6139127550.24 & -789725025.00 \\ 532719070.00 & 483911309.20 & 167860800.00 \\ 493965108.00 & -425680179.12 & 297487890.00 \\ 904386900.00 & 1322148144.00 & 314293500.00 \\ -1003345536.00 & -590256150.96 & -1404372330.00 \\ -426175256.00 & -387129047.36 & -134288640.00 \\ -213087628.00 & -193564523.68 & -67144320.00 \end{bmatrix}$$

Required vectors  $y$  and  $x$ , according to (4.12) and (4.13) are

$$y = (I - G^+ G)u = \begin{bmatrix} 1.2365580746 \\ 0.9079895101 \\ 0.1459498604 \\ 1.0653080872 \\ 0.5435245343 \\ 1.0866921189 \end{bmatrix}$$

$$\text{and } x = A^+ B y - (I - A^+ A)v = \begin{bmatrix} 1.0653080872 \\ 0.0208499800 \\ 0.0320088416 \\ 1.2365580746 \\ 0.9079895101 \end{bmatrix}$$

Now immediately follows balanced equation in its conventional form



According to the definition 3. 6, extended matrix obtains the form

$$\text{Ext}A|B = \begin{bmatrix} 1 & 0.00 & 0.00 & 0 & 0 & 0 & 0.00 & 1 & 0.00 & 0 \\ 2 & 18.0 & 0.00 & 2 & 0 & 2 & 6.00 & 0 & 1.00 & 1 \\ 3 & 0.00 & 50.0 & 0 & 0 & 3 & 0 & 0.00 & 0 & 0.00 & 1 \\ 1 & 0.00 & 0.00 & 0 & 0 & 0 & 0.00 & 0 & 1.96 & 0 \\ 3 & 0.00 & 15.0 & 6 & 2 & 3 & 3 & 0.00 & 2 & 2.00 & 3 \\ 0 & 7.00 & 0.00 & 0 & 0 & 0 & 1.00 & 0 & 0.00 & 0 \\ 0 & 18.0 & 44.0 & 0 & 0 & 0 & 1 & 6.00 & 0 & 0.00 & 0 \\ 0 & 0.00 & 0.00 & 1 & 0 & 1 & 0 & 0.00 & 0 & 0.00 & 0 \\ 0 & 0.00 & 0.00 & 0 & 2 & 1 & 0 & 3.97 & 0 & 0.00 & 0 \\ 0 & 0.00 & 0.00 & 0 & 1 & 0 & 1 & 0.00 & 0 & 0.00 & 0 \\ 0 & 0.00 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0 & 0.00 & 1 \end{bmatrix}$$

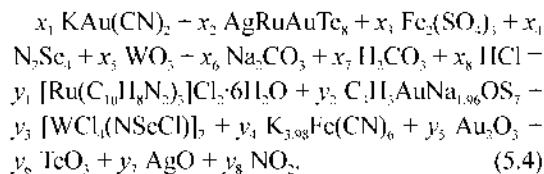
The eigenvalues of the matrix  $[\text{Ext}A|B + (\text{Ext}A|B)^T]/2$  are  $\lambda_1=59.824, \lambda_2=21.786, \lambda_3=-10.767, \lambda_4=5.648, \lambda_5=-4.030, \lambda_6=-2.045, \lambda_7=-0.940, \lambda_8=-0.044, \lambda_9=-1.678, \lambda_{10}=-0.831, \lambda_{11}=-1.059$ .

The Lozinskiĭ measures of  $\text{Ext}A|B$  given by (3.6) with respect to the three common norms (3.5) are

$$\begin{aligned} \mu_1(\text{Ext}A|B) &= \max(2, 32, 57, 2.96, 39, 8, 69, 2, 6.97, 2, 1) = 69, \\ \mu_2(\text{Ext}A|B) &= \max(10, 43, 109, 9, 5, 10, 5, 16.97, 3, 4.96, 6) = 109, \\ \mu_3\{[\text{Ext}A|B + (\text{Ext}A|B)^T]/2\} &= 59.824. \end{aligned}$$

Since  $\mu_2\{[\text{Ext}A|B + (\text{Ext}A|B)^T]/2\} > 0$ , according to the definition 4.5 the chemical equation (5.3) is unstable.

**Example 5. 4.** We will now balance this equation



The matrix of reactants *A* is

	$\text{KAu(CN)}_2$	$\text{AgRuAuTe}_k$	$\text{Fe}_2(\text{SO}_4)_3$	$\text{N}_2\text{Se}_4$	$\text{WO}_3$	$\text{Na}_2\text{CO}_3$	$\text{H}_2\text{CO}_3$	$\text{HCl}$	
<i>A</i>	1	0	0	0	0	0	0	0	K
	1	1	0	0	0	0	0	0	Au
	2	0	0	0	0	1	0	0	C
	2	0	0	2	0	0	0	0	N
	0	1	0	0	0	0	0	0	Ag
	0	1	0	0	0	0	0	0	Ru
	0	8	0	0	0	0	0	0	Te
	0	0	2	0	0	0	0	0	Fe
	0	0	3	0	0	0	0	0	S
	0	0	12	0	3	3	3	0	O
	0	0	0	4	0	0	0	0	Se
	0	0	0	0	1	0	0	0	W
	0	0	0	0	0	2	0	0	Na
	0	0	0	0	0	0	2	1	H
	0	0	0	0	0	0	0	1	Cl

and the matrix of the products *B* is

	$[\text{Ru}(\text{C}_{10}\text{H}_8\text{N}_2)_2]\text{Cl}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}_7\text{H}_7\text{AuNa}_{1.96}\text{OS}_7$	$[\text{WCl}_4(\text{NSeCl})_2]_2$	$\text{K}_{3.98}\text{Fe(CN)}_6$	$\text{Au}_5\text{O}_3$	$\text{TeO}_3$	$\text{AgO}$	$\text{NO}_2$	
<i>B</i>	0	0	0	3.98	0	0	0	0	K
	0	1	0	0	2	0	0	0	Au
	36	4	0	0	0	0	0	0	C
	6	0	2	0	0	0	0	1	N
	0	0	0	0	0	0	1	0	Ag
	1	0	0	0	0	0	0	0	Ru
	0	0	0	0	0	1	0	0	Te
	0	0	0	1	0	0	0	0	Fe
	0	7	0	0	0	0	0	0	S
	6	1	0	0	3	3	1	2	O
	0	0	2	0	0	0	0	0	Se
	0	0	2	0	0	0	0	0	W
	0	1.96	0	0	0	0	0	0	Na
	36	3	0	0	0	0	0	0	H
	2	0	10	0	0	0	0	0	Cl

The reaction matrix *A|B*, according to the defini-

tion 3.5 obtains this form

$$A|B = \begin{bmatrix} 1 & 0 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 3.98 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 1.00 & 0.00 & 0.00 & 2 & 0 & 0 & 0 \\ 2 & 0 & 0.00 & 0 & 0 & 1 & 1 & 0 & 30.0 & 4.00 & 0.00 & 6.00 & 0 & 0 & 0 \\ 2 & 0 & 0.00 & 2 & 0 & 0 & 0 & 0 & 6.00 & 0.00 & 2.00 & 6.00 & 0 & 0 & 1 \\ 0 & 1 & 0.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 0.00 & 0 & 0 & 1 \\ 0 & 1 & 0.00 & 0 & 0 & 0 & 0 & 0 & 1.00 & 0.00 & 0.00 & 0.00 & 0 & 0 & 0 \\ 0 & 8 & 0.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 0.00 & 0 & 1 & 0 \\ 0 & 0 & 2.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 1.00 & 0 & 0 & 0 \\ 0 & 0 & 3.00 & 0 & 0 & 0 & 0 & 0 & 0.00 & 7.00 & 0.00 & 0.00 & 0 & 0 & 0 \\ 0 & 0 & 12.0 & 0 & 3 & 3 & 3 & 0 & 6.00 & 1.00 & 0.00 & 0.00 & 3 & 3 & 1 \\ 0 & 0 & 0.00 & 4 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 2.00 & 0.00 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 1 & 0 & 0 & 0 & 0.00 & 0.00 & 2.00 & 0.00 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 2 & 0 & 0 & 0.00 & 1.96 & 0.00 & 0.00 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 0 & 1 & 2 & 36.0 & 3.00 & 0.00 & 0.00 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 0 & 0 & 1 & 2.00 & 0.00 & 10.0 & 0.00 & 0 & 0 & 0 \end{bmatrix}$$

The rank of the above matrix is  $\rho = 15$ . Since the nullity of the reaction matrix is  $\kappa - r + s - \rho = 8 + 8 - 15 = 1$ , then we have only a unique solution, that means that the reaction is feasible. Next, we will determine the solution *x*, *y*.

The Moore-Penrose pseudoinverse  $A^+ = (A^T A)^{-1} A^T$  of the matrix *A* is

94083728 *A*<sup>+</sup> =

12161840	11980320	15511840	19458944	-181520	-181520	-1452160	2315520
-181520	1225424	-231520	-290432	1406944	1406944	11255552	-34560
1157760	1140480	-3001536	1852416	-17280	-17280	-138080	8264608
-2432384	-2346064	-3102368	5516584	36304	36304	290432	-463104
3762720	3706560	-9754992	6020352	-56160	-56160	-449280	-3484800
-2937280	-2893440	7615008	-4699648	43840	43840	350720	-3544704
-5874560	-5786880	15230016	-9399296	87680	87680	701440	-7089408
5874560	5786880	-15230016	9399296	-87680	-87680	-701440	7089408
3473280	-1254240	-9729472	3762720	-5874560	-5874560	5874560	-31840
-31840	18720	145216	-56160	87680	87680	-87680	12396912
12396912	3363648	-926208	-10090944	-4544704	-4544704	-3544704	3544794
-694656	-250848	20762640	-752544	1174912	1174912	-1174912	-30272832
-30272832	10931856	-3010176	61288160	-11520288	-11520288	11520288	-5317056
-5317056	1920048	2349824	-5760144	40354288	-6687576	6687576	10634112
10634112	3840096	4699648	11520288	13375152	33666712	-33666712	10634112
10634112	-3840096	-4699648	11520288	13375152	13375152	80708576	

and the matrix *G* has this form

94083728 *G* = (94083728 *I* - *AA*<sup>+</sup>)*B* =

-374666864.00	-67948582.40	-85729984.00	113908890.24
-370479056.00	25745068.80	-84450432.00	-256655625.60
520438048.00	129819488.64	146991200.00	36642428.80
-147865088.00	-108717731.84	-61900992.00	34730938.88
4187808.00	-390076.80	1279552.00	3888721.60
98271536.00	-390076.80	1279552.00	3888721.60
33502464.00	-3120614.40	10236416.00	31109772.80
358573824.00	-123389272.32	-34235136.00	82128182.40
537860736.00	473502187.52	-51352704.00	-17933318.40
-194227488.00	-97810668.16	18544032.00	-9204700.80
73932544.00	54358865.92	30950496.00	-17365469.44
582682464.00	293432004.48	-55632096.00	27614102.40
31122208.00	81806257.92	-101311648.00	-4514163.20
31122208.00	81806257.92	-101311648.00	-4514163.20
-31122208.00	-81806257.92	101311648.00	4514163.20

-20197920.00	5214880.00	1435760.00	-16950464.00
165462528.00	-6096832.00	10096.00	-16697472.00
-40315632.00	-7902832.00	-3020144.00	-31322272.00
-32316672.00	8343808.00	2297216.00	48146240.00
-2507008.00	-11311712.00	92658064.00	252992.00
-2507008.00	-11311712.00	-1425664.00	252992.00
-20056064.00	3590032.00	-11405312.00	2023936.00
-24743808.00	-19905408.00	-6692736.00	-17159424.00
-37115712.00	-29858112.00	-10039104.00	-25739136.00
13402896.00	10782096.00	3625232.00	9294688.00
16158336.00	-4171904.00	-1148608.00	-24073120.00
-40208688.00	-32346288.00	-10875696.00	-27884064.00
53472.00	-12221728.00	-3927776.00	1719104.00
53472.00	-12221728.00	-3927776.00	1719104.00
-53472.00	12221728.00	3927776.00	-1719104.00

obtains the form

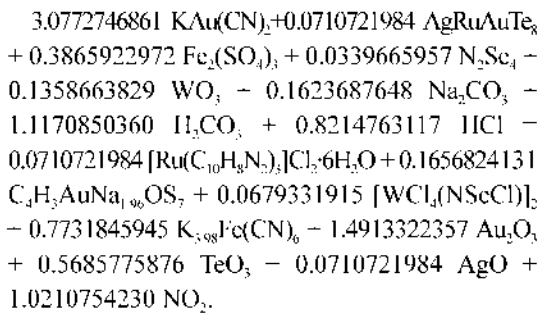
$$\text{Ext}A_1B = \begin{bmatrix} 0 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 3.98 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0.00 & 0 & 0 & 0 & 0.00 & 1.00 & 0.00 & 0.00 & 2 & 0 & 0 & 0 \\ 2 & 0 & 0.00 & 0 & 0 & 1 & 1 & 0 & 30.0 & 4.00 & 0.00 & 6.00 & 0 & 0 & 0 \\ 2 & 0 & 0.00 & 2 & 0 & 0 & 0 & 6.00 & 0.00 & 2.00 & 6.00 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 0.00 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0.00 & 0 & 0 & 0 & 0 & 1.00 & 0.00 & 0.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 8 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 0.00 & 0 & 1 & 0 & 0 \\ 0 & 0 & 2.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 1.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3.00 & 0 & 0 & 0 & 0 & 0.00 & 7.00 & 0.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 12.0 & 0 & 3 & 3 & 3 & 6.00 & 1.00 & 0.00 & 0.00 & 3 & 3 & 1 & 2 \\ 0 & 0 & 0.00 & 4 & 0 & 0 & 0 & 0.00 & 0.00 & 2.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 1 & 0 & 0 & 0.00 & 0.00 & 2.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 2 & 0 & 0.00 & 1.96 & 0.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 2 & 1 & 36.0 & 3.00 & 0.00 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 0 & 1 & 2.00 & 0.00 & 10.0 & 0.00 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.00 & 0 & 0 & 0 & 0 & 0.00 & 0.00 & 0.00 & 0.00 & 0 & 0 & 0 & 1 \end{bmatrix}$$

Required vectors  $y$  and  $x$ , according to (4.12) and (4.13) are

$$y = (I - G^*G)u = \begin{bmatrix} 0.0710721984 \\ 0.1656824131 \\ 0.0679331915 \\ 0.7731845945 \\ 1.4913322357 \\ 0.5685775876 \\ 0.0710721984 \\ 1.0210754230 \end{bmatrix}$$

$$\text{and } x = A^1B y + (I - A^1A)v = \begin{bmatrix} 3.0772746861 \\ 0.0710721984 \\ 0.3865922972 \\ 0.0339665957 \\ 0.1358663829 \\ 0.1623687648 \\ 1.1170850360 \\ 0.8214763117 \end{bmatrix}$$

Now immediately follows balanced equation in its conventional form



According to the definition 3. 6. extended matrix

The eigenvalues of the matrix  $[\text{Ext}A_1B + (\text{Ext}A_1B)^1]/2$  are  $\lambda_1 = -28.656$ ,  $\lambda_2 = -24.826$ ,  $\lambda_3 = -9.278$ ,  $\lambda_4 = -6.650$ ,  $\lambda_5 = -6.847$ ,  $\lambda_6 = 5.301$ ,  $\lambda_7 = 4.806$ ,  $\lambda_8 = 3.495$ ,  $\lambda_9 = -3.389$ ,  $\lambda_{10} = -2.805$ ,  $\lambda_{11} = 1.297$ ,  $\lambda_{12} = -0.937$ ,  $\lambda_{13} = 0.759$ ,  $\lambda_{14} = -0.312$ ,  $\lambda_{15} = 0.040$ ,  $\lambda_{16} = 0.134$ .

The Lozinskiĭ measures of  $\text{Ext}A_1B$  given by (3.6) with respect to the three common norms (3.5) are

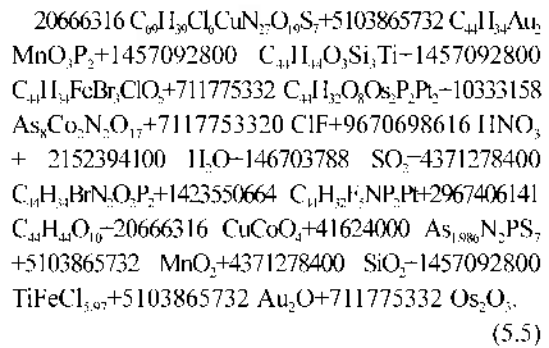
$$\mu_1(\text{Ext}A_1B) = \max(4.98, 5, 44, 19, 2, 2, 9, 3, 10, 37, 6, 3, 3.96, 42, 13, 1) = 44,$$

$$\mu_2(\text{Ext}A_1B) = \max(6, 11, 17, 6, 4, 6, 6, 2, 81, 17.96, 16, 16.98, 5, 4, 2, 4) = 81,$$

$$\mu_2\{[\text{Ext}A_1B + (\text{Ext}A_1B)^1]/2\} = 28.656.$$

Since  $\mu_2\{[\text{Ext}A_1B + (\text{Ext}A_1B)^1]/2\} > 0$ , according to the definition 4. 5 the chemical equation (5.4) is unstable.

**Example 5. 5.** Also, we balanced this very interesting chemical equation



According to the definition 3. 6. extended matrix

obtains the form

$$\text{Ext}A|B = \begin{bmatrix} 69.44 & 44.44 & 44.44 & 0 & 0 & 0 & 0 & 44.44 & 44.44 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 39.34 & 44.34 & 34.32 & 0 & 0 & 1 & 2 & 0 & 34.32 & 44.0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 \\ 27 & 0 & 0 & 0 & 0 & 2 & 0 & 1 & 0 & 0 & 2.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 19 & 3 & 3 & 5 & 8 & 17 & 0 & 3 & 1 & 2 & 2 & 0 & 1 & 0 & 4 & 0.000 & 2 & 2 & 0 & 0 & 0 & 1 & 3 \\ 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 1.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.986 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 7 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 7.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 5.97 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.000 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

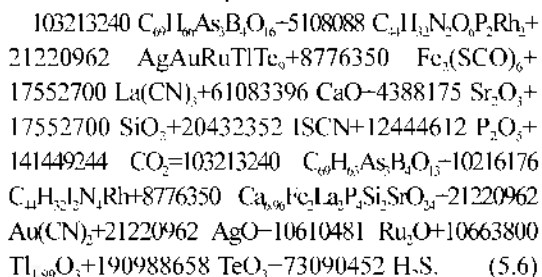
The eigenvalues of the matrix  $[\text{Ext}A|B + (\text{Ext}A|B)^t]/2$  are  $\lambda_1=143.364$ ,  $\lambda_2=-41.450$ ,  $\lambda_3=14.630$ ,  $\lambda_4=-11.150$ ,  $\lambda_5=11.154$ ,  $\lambda_6=-6.730$ ,  $\lambda_7=4.060$ ,  $\lambda_8=-3.424$ ,  $\lambda_9=-3.357$ ,  $\lambda_{10}=-3.432$ ,  $\lambda_{11}=-2.112$ ,  $\lambda_{12}=-2.481$ ,  $\lambda_{13}=-1.348$ ,  $\lambda_{14}=-1.453$ ,  $\lambda_{15}=-0.544$ ,  $\lambda_{16}=-0.614$ ,  $\lambda_{17}=-0.575$ ,  $\lambda_{18}=-0.137$ ,  $\lambda_{19}=-0.090$ ,  $\lambda_{20}=-0.006$ .

The Lozinskiĭ measures of  $\text{Ext}A|B$  given by (3.6) with respect to the three common norms (3.5) are

$$\begin{aligned} \mu(\text{Ext}A|B) &= \max(377, 296, 4, 35, 85, 9, 6, 3, 2, 3, 9.986, 15, 2, 4, 2, 2, 13.97, 4, 4, 1) = 377, \\ \mu_1(\text{Ext}A|B) &= \max(168, 86, 95, 88, 90, 29, 2, 5, 3, 3, 85, 85, 98, 6, 11.986, 3, 3, 7.97, 3, 6) = 168, \\ \mu_2\{[\text{Ext}A|B + (\text{Ext}A|B)^t]/2\} &= 143.364. \end{aligned}$$

Since  $\mu_2\{[\text{Ext}A|B + (\text{Ext}A|B)^t]/2\} > 0$ , according to the definition 4.5 the chemical equation (5.5) is unstable.

**Example 5.6.** An other chemical equation which we balanced is the equation



The reaction matrix  $A|B$ , according to the defini-

tion 3.5 has the form

$$A|B = \begin{bmatrix} 69.44 & 0 & 6 & 3 & 0 & 0 & 0 & 1 & 0 & 1 & 69.44 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 66.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 63.32 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 16 & 6 & 0 & 6 & 0 & 1 & 3 & 2 & 0 & 5 & 2 & 13 & 0 & 24 & 0 & 1 & 1 & 3 & 3 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 4 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1.99 & 0 & 0 & 0 & 0 \\ 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6.96 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

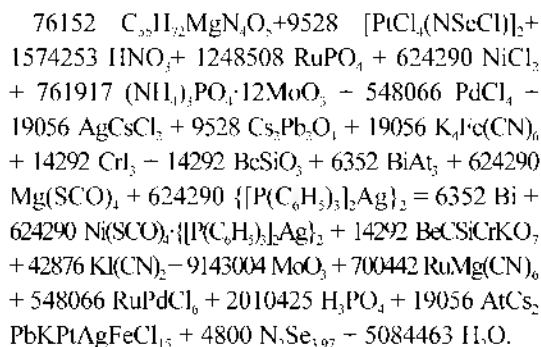
The eigenvalues of the matrix  $[A|B - (A|B)^t]/2$  are  $\lambda_1=131.840$ ,  $\lambda_2=-24.264$ ,  $\lambda_3=15.402$ ,  $\lambda_4=-13.779$ ,  $\lambda_5=-8.097$ ,  $\lambda_6=4.189$ ,  $\lambda_7=3.564$ ,  $\lambda_8=-3.485$ ,  $\lambda_9=-2.396$ ,  $\lambda_{10}=-1.459$ ,  $\lambda_{11}=-1.347$ ,  $\lambda_{12}=-1.023$ ,  $\lambda_{13}=-0.923$ ,  $\lambda_{14}=-0.748$ ,  $\lambda_{15}=-0.449$ ,  $\lambda_{16}=-0.722$ ,  $\lambda_{17}=-0.513$ ,  $\lambda_{18}=-0.116$ ,  $\lambda_{19}=-0.011$ ,  $\lambda_{20}=-0.075$ .

The Lozinskiĭ measures of  $A|B$  with respect to the three common norms are

$$\begin{aligned} \mu(A|B) &= \max(239, 195, 6, 8, 86, 12, 8, 3, 2, 2, 3, 2.99, 10, 4, 8, 3, 7.96, 3, 3, 3) = 239, \\ \mu_1(A|B) &= \max(158, 88, 13, 20, 7, 2, 5, 3, 4, 7, 3, 152, 83, 41.96, 5, 2, 3, 4.99, 4, 3) = 158, \\ \mu_2\{[A|B - (A|B)^t]/2\} &= 131.840. \end{aligned}$$

Because  $\mu_2\{[A|B - (A|B)^t]/2\} > 0$ , that means that the chemical equation (5.6) is unstable.

**Example 5.7.** It will be benefit for us if we balance some little bit bigger chemical equation, for instance like this





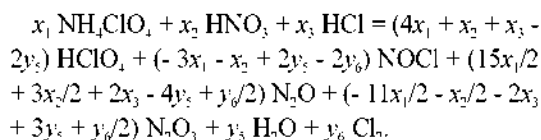
$$\begin{aligned}4x_1 + x_2 + x_3 &= y_1 + 2y_5, \\x_1 + x_3 &= y_1 + y_2 + 2y_6, \\4x_1 + 3x_2 &= 4y_1 + y_2 + y_3 + 3y_4 + y_5.\end{aligned}$$

The general solution of the above system is

$$\begin{aligned}y_1 &= 4x_1 + x_2 + x_3 - 2y_5, y_2 = -3x_1 - x_2 + 2y_5 - 2y_6, \\y_3 &= 15x_1/2 + 3x_2/2 + 2x_3 - 4y_5 + y_6/2, \\y_4 &= -11x_1/2 - x_2/2 - 2x_3 + 3y_5 + y_6/2.\end{aligned}$$

where  $x_1, x_2, x_3, y_5$  and  $y_6$  are arbitrary real numbers.

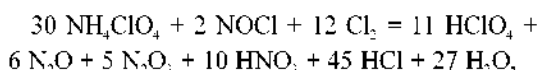
Now, the balanced equation has a form



where  $x_1, x_2, x_3, y_5$  and  $y_6$  are arbitrary real numbers.

A particular case of equation (5.10) for  $y_4=0$  is solved in<sup>8</sup>, but there the author balanced this equation on completely different way by using of non-singular matrix method. So, it is the mathematical consideration of this equation, but for chemical purposes stoichiometric coefficients must be unique.

Now, if we employ here offered method we obtain that only possible chemical equation is this equation



which actually is a particular case of the chemical equation (5.10) for  $x_1=1, x_2=-1/3, x_3=-3/2, y_5=9/10$  and  $y_6=-2/5$ .

Also, in the article<sup>78</sup>, is balanced a particular case for  $x_1=34, x_2=36, x_3=8$ , and  $y_5=y_6=0$ .

## 6. CONCLUSION

The practical power of the matrix procedure as the most general tool for balancing chemical equations is demonstrable. By this method are balanced

completely new classes of chemical equations with atoms, which have fractional oxidation numbers. Research shown that employed pseudoinverse matrix method founded on virtue of the solution of the Diophantine matrix equation works perfectly for the all chemical equations.

Actually, this method is unique method both in mathematics and chemistry, which generalize to date the all known methods and particular techniques for balancing chemical equations cited in the bibliography given below. In other words speaking, the mathematical method given here is applicable for the all possible cases for balancing chemical equations, does not matter what kind of atoms they possess – fractional or integer oxidation numbers. Also, this method determine and  $r + s - \rho$  linear independent solutions when  $\kappa > 1$ , i.e., when the reaction is feasible and is non-unique. This is the main advantage of the method in relation of other known particular methods and techniques.

For all considered chemical equations which have a unique solution is made stability analysis, and as shown results all of them are unstable. This stability analysis is founded on virtue of the Lozinski measures of extended matrix.

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