A New Singular Matrix Method for Balancing Chemical Equations and Their Stability

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>Only the matrix method is powerful enough to balance the skeletal chemical equation.«

In this work is given a new singular matrix method for balancing new classes of chemical equations which reduce to an $n \times n$ matrix. The method offered here is founded by virtue of the solution of a homogeneous matrix equation by using of Drazin pseudoinverse matrix. The method has been tested on many typical chemical equations and found to be very successful for the all equations in our extensive balancing research. This method works successfully without any limitations. Chemical equations treated here possess atoms with fractional oxidation numbers. Also, in the present work are analyzed some necessary and sufficient criteria for stability of chemical equations over stability of their reaction matrices.

Keywords: Mathematical method; Matrices; Balancing chemical equations; Stability.

1. INTRODUCTION

What it is a chemical equation? Briefly speaking, a chemical equation is only a symbolic representation of a chemical reaction. Actually, every chemical equation is the story of some chemical reaction. 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 researcher, 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. Chemical equations play a main role in theoretical as well as industrial chemistry. Mass balance of chemical equations as a century old problem is one of the most highly studied topics in chemical education. It always has the biggest interest for the students and the teachers as well on every level as a magic topic. Also, for qualitative and quantitative understanding of the chemical process estimating reactants, predicting the nature and amount of products and determining reaction conditions is necessary a balanced chemical equation. Every student who has general chemistry as a subject is bound to come across balancing chemical equations. Actually, balancing chemical equations provides an excellent demonstrative and pedagogical example of interconnection between stoichiometrical principles and linear algebra.

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.

In other words, a chemical equation should represent the stoichiometry observed in the chemical reaction. 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 very 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 there exists only a trivial solution, i.e., all coefficients are equal to zero.

2. HISTORICAL BACKGROUND

The main purpose in this section is to gives a survey...
of selected articles on balancing chemical equations that may be useful to chemistry teachers and potential authors as background material, and to provide some comparisons of methods. The selection criteria for references were intentionally wide, in order to include a large variety of topics and former historical citations.

Balancing chemical equations in the scientific literature is considered from four points of view: mathematical, computational, chemical and pedagogical.

Now, briefly we will describe these views.

- Jones for the first time in mathematics proposed the general problem for balancing chemical equations. Actually he formalized a century old problem in a compact linear operator form as a Diophantine matrix equation. After that, Krishnamurthy gave a mathematical method for balancing chemical equations founded by virtue of a generalized matrix inverse. He considered some elementary chemical equations, which were well-known in chemistry for a long time. A little bit later Das offered a simple mathematical method, which was discussed in the ref. A computer model for balancing some elementary chemical equations over an integer programming approach is given in the ref. In the article by use of a reflexive $g$-inverse matrix is solved the general problem of balancing chemical equations proposed in the ref. Other mathematical results for balancing chemical equations and their stability over a nonsingular matrix method are obtained in the ref. Last, the most general results for balancing chemical equations over a Moore-Penrose pseudoinverse matrix are obtained in the ref. Actually, to date in mathematics and chemistry there are only four strictly formalized consistent mathematical methods for balancing chemical equations; they are methods given in the ref. and the method presented in this work, while other so called methods in chemical sense have limited usage, and they are useful only for particular cases, especially for balancing chemical equations which possess atoms with integer oxidation numbers.

- There are many published articles in chemistry, which consider the use of computers to balancing chemical equations. All of these computational methods use some commercial software packet, but unfortunately none of them deals with fractional oxidation numbers. That is one of their biggest weaknesses, which limits them to be applicable only in some particular cases and nothing more. It is of interest to emphasize here that the same holds for the current online methods available on the internet which employ only integer oxidation numbers. So, to date we do not know any computer method for balancing chemical equations to deal with fractional oxidation numbers, except previously mentioned methods of the author of this work. Actually, it was the main motive for the author to direct his research for development of new mathematical methods for balancing chemical equations in $\mathbb{Q}$ (the set of rational numbers of the form $p/q$) in such a way to extend and generalize the current particular techniques used in chemistry right now for balancing only chemical equations in $\mathbb{N}$ (the set of natural numbers).

- 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.

Several simple chemical equations are solved by elementary algebraic techniques in the ref. The earliest article that makes use of the linear algebra method was published by Bottomley. A set of various modifications which implement this approach is documented in the ref. The case when the chemical equation has no unique solution received considerable attention in the education articles. The equation represents two or more independently occurring reactions can be combined in varying stoichiometric ratios. Fixed ratios of reagents, observed experimentally in particular cases, are equivalent to a restriction on the coefficients that make a unique solution.

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. The valence change method and the ion-electron method 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 emphasis that first Karslake in the ref. considered balancing of ionic chemical equations. Actually, the technique suggested by Garcia can reduce the number of algebraic steps for ion-electron method. Previous 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\textsuperscript{115} defined the equivalent term oxidation stage change on this subject.

Stout in the ref.\textsuperscript{116} 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.\textsuperscript{117-122}

- Balancing chemical equations through the pedagogical point of view is given in the articles.\textsuperscript{111,123-130} This approach is very interesting for the education of chemical research. A check of the hypothesis that formal reasoning and 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.\textsuperscript{130}

3. PRELIMINARIES

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

**Definition 3.1.** For the matrix \( A \in \mathbb{R}^{n \times n} \), the smallest nonnegative integer \( i \) such that
\[
\text{rank}(A^i) = \text{rank}(A^{i+1}),
\]
is called the index of \( A \), and is denoted by \( \text{Ind}(A) = i \).

**Definition 3.2.** The Drazin inverse \( A^D \) of a matrix \( A \in \mathbb{R}^{n \times n} \) with \( \text{Ind}(A) = i \), is the unique matrix satisfying the following criteria
\[
AA^D = A^DA, A^DAA^D = A^D, A^{i+1}A^D = A^i.
\]

Pseudoinverse matrix \( A^D \) of a matrix \( A \) was defined by Drazin.\textsuperscript{131}

**Definition 3.3.** When \( \text{Ind}(A) = 1 \), if the matrix \( A^D \) satisfies (3.2), then it is called the group inverse of \( A \), denoted by \( A^* \).

**Remark 3.4.** If \( A \) is nonsingular, then it is easily seen that \( \text{Ind}(A) = 0 \), and \( A^{-1} = A^D \) satisfies (3.2), i.e., \( A^D = A^{-1} \).

**Definition 3.5.** The characteristic equation of an \( n \times n \) matrix \( A \) is the equation in one variable \( \lambda \)
\[
det(\lambda I - A) = 0,
\]
where \( \det(\cdot) \) denotes a determinant and \( I \) is an \( n \times n \) identity matrix.

**Definition 3.6.** The polynomial
\[
p(\lambda) = \det(\lambda I - A) = \lambda^n + a_1\lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n
\]
which results from evaluating the determinant (3.3) is the characteristic polynomial of the matrix \( A \).

**Definition 3.7.** The roots of the characteristic polynomial (3.4) are precisely the eigenvalues of the matrix \( A \).
Let \( \sigma(A) = \{ \lambda_i, 1 \leq i \leq n \} \) be the spectrum of \( A \).

The polynomial (3.4) of degree \( n \geq 1 \) with real coefficients \( a_i (1 \leq i \leq n) \), by the fundamental theorem of algebra has \( n \) (not necessarily distinct) roots \( \lambda_1, \lambda_2, \ldots, \lambda_n \).

The Souriau-Frame algorithm\textsuperscript{132,133} permits simultaneous determination of the coefficients \( a_i (1 \leq i \leq n) \) in (3.4) and the matrices \( B_j (1 \leq j \leq n-1) \) in the following expression
\[
(\lambda I - A)^{-1} = (\lambda^n I + \lambda^{n-2} B_1 + \cdots + \lambda B_{n-2} + B_{n-1})/p(\lambda),
\]
by means of the recursive formulae
\[
a_1 = -\text{tr}(A), \quad B_1 = A + a_1I, \quad B_p = -(\text{tr}\ AB_{p-1})/(2 \leq p \leq n),
\]
\[
B_p = AB_{p-1} + a_pI, \quad B_n = OA = AB_{n-1} + a_nI,
\]
where \( \text{tr}(A) \) denotes the trace of \( A \) and \( O \) is an \( n \times n \) zero matrix.

If \( A \) is a nonsingular matrix, then \( a_n \neq 0 \). It is very easy to see that from (3.8) follows
\[
A^{-1} = -B_{n-1}/a_n.
\]

Greville’s finite algorithm\textsuperscript{134} for Drazin inverse of an \( n \times n \) matrix is a natural extension of the above result for \( A^{-1} \).

**Definition 3.8.** For any matrix \( A \in \mathbb{R}^{n \times n} \) we denote \( \text{Im}A \) \( \{ y \in \mathbb{R}^n : y = Ax \} \) the image of \( A \) or range of \( A \).

**Definition 3.9.** For any matrix \( A \in \mathbb{R}^{n \times n} \) we denote \( \text{Ker}A \) \( \{ x \in \mathbb{R}^n : Ax = 0 \} \) the kernel of \( A \) or null space of \( A \).

**Definition 3.10.** nullity\( A = \dim(\text{Ker}A) \).

**Definition 3.11.** \( \text{rank}A = \dim(\text{Im}A) \).

Let \( \text{rank}A = r \) and let nullity\( A = k \). According to the ref.\textsuperscript{135} the deterministic approach is important, since it enables us to classify the chemical reaction as:

1. \( 1^o \) infeasible when the nullity of the reaction matrix is zero;
2. \( 2^o \) unique (within relative proportions) when the nullity of the reaction matrix is one; or
3. \( 3^o \) non-unique when its nullity is bigger than one.

Possible cases of balancing chemical equations are the following

1. If \( r = n \) then \( k = n - r = 0 \), i.e., trivial solution \( x = 0 \), the reaction is infeasible.
2. If \( r = n - 1 \), then \( k = n - r = 1 \), unique solution \( x \neq 0 \), 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 \( r < n - 1 \), then \( k = n - r > 1 \), \( k (> 1) \) linearly independent solutions \( x \neq 0 \), i.e., the reaction is feasible and is non-unique.

Last kind 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.

Let \( | \cdot | \) denotes a vector norm in \( \mathbb{R}^n \).

**Definition 3.12.** The Lozinskii measure \( \mu \) on \( \mathbb{R}^n \) with respect to \( | \cdot | \) is defined by

\[
\mu(A) = \lim_{\rho \to 0^+} \frac{(I + \rho A) - 1}{\rho}. \tag{3.10}
\]

**Definition 3.13.** The Lozinskii measures of \( A = [a_{ij}]_{n \times n} \) with respect to the three common norms

\[
| x |_1 = \sum_i | x_i |,
\]

\[
| x |_2 = (\sum_i | x_i |^2)^{1/2},
\]

are

\[
\mu_1(A) = \sup_i (\sum_j | a_{ij} |),
\]

\[
\mu_2(A) = \sup_i (\sum_j | a_{ij} |),
\]

\[
\mu_3(A) = \text{stab}(A^T), \quad \text{(3.12)}
\]

where

\[
\text{stab}(A) = \max \{ \lambda, \lambda \in \sigma(A) \}
\]

is the stability modulus of \( A \) and \( T \) denotes transpose.

**Definition 3.14.** The matrix \( A \) is stable if \( \text{stab}(A) < 0 \).

4. MAIN RESULTS

In this section we will give a completely new method for balancing 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

\[
\sum_{j=1}^{n} x_j \prod_{i=1}^{m} \Psi_{aij} = 0, \tag{4.1}
\]

where \( x_j (1 \leq j \leq n) \) are unknown rational coefficients, \( \Psi^i (1 \leq i \leq n) \) are chemical elements and \( a_{ij} (1 \leq i, j \leq n) \) are numbers of atoms of element \( \Psi^i \) in \( j \)-th molecule.

**Proof.** Let there exists an arbitrary chemical equation from \( n \) distinct elements and \( n \) molecules

\[
\sum_{j=1}^{n} x_j \Phi_j = 0, \tag{4.2}
\]

where \( \Phi_j = \Psi^1_{aij} \Psi^2_{aj} \cdots \Psi^m_{aj} (1 \leq j \leq n) \). Then previous expression becomes

\[
\sum_{j=1}^{n} x_j \Psi^1_{aij} \Psi^2_{aj} \cdots \Psi^m_{aj} \Phi_j = 0. \tag{4.3}
\]

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

The coefficients satisfy three basic principles (corresponding to a closed input-output static model\(^{136,137}\))

- 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 matrix equation

\[
Ax = 0, \tag{4.4}
\]

where \( A = [a_{ij}]_{n \times n} \) is a reaction matrix, \( x^T = (x_1, x_2, \ldots, x_n) \) is a column vector of the coefficients \( x_j (1 \leq j \leq n) \) and \( 0^T = (0, 0, \ldots, 0) \) is a null column vector of order \( n \) and \( T \) denotes transpose.

**Proof.** If we develop the molecules of the reaction (4.1) in an explicit form, then we obtain the reaction matrix \( A \) shown below

\[
\Phi_j = \sum_{i=1}^{n} a_{ij} \Psi^i (1 \leq j \leq n). \tag{4.5}
\]

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

\[
\sum_{j=1}^{n} x_j \sum_{i=1}^{n} a_{ij} \Psi^i = 0, \tag{4.6}
\]

or

\[
\sum_{i=1}^{n} \Psi^i \sum_{j=1}^{n} a_{ij} x_j = 0, \tag{4.7}
\]

i.e.,
\[
\sum_{j=1}^{n} a_j x_j = 0 \quad (1 \leq i \leq n).
\]  \hspace{1cm} (4.8)

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 \( p \) in (3.7) be the largest integer such that \( a_p \neq 0 \). Then the Drazin pseudoinverse \( A^p \) of \( A \) is
\[
A^p = (-1)^{m+1}A^n(B_{p+1}/a_p)^{m+1}, \quad \forall m \geq i = \text{Ind}(A).
\]  \hspace{1cm} (4.9)

**Proof.** If \( i = 0 \), then the matrix \( A \) is nonsingular and \( a_n \neq 0 \). Also, it is known that \( A \) and each \( B_p \) commute. Taking into account the second expression of (3.8) we have
\[
A^p(B_{p+1})^n = (-1)^{m+1}(a_p)^n, \quad m \geq 0.
\]
Using the result in (3.9), we have
\[
A^p = A^1 - (B_{p+1}/a_p) = (-1)^{m+1}A^n(B_{p+1}/a_p)^{m+1}.
\]
If \( i > 0 \), then \( m \geq i \geq 1 \). By the definition of \( p \) and (3.8) we obtain
\[
AB_{p+1} = O \quad \text{and} \quad AB_j = AB_{j+1} \quad (p + 1 \leq j \leq n - 1),
\]
which further imply
\[
A^nB_{p+1} = O \quad \text{and} \quad A^nB_j = A^{n+1}B_{j+1}, \quad (n - 1 \leq j \leq p + 1). \quad (4.10)
\]
We suppose that \( A^nB_j = O \). From this case in (4.10) follows a new expression
\[
A^nB_j = O \quad (n - 1 \leq j \leq p + 1). \quad (4.11)
\]
Thus, we obtain
\[
A^nB_{p+1} = (A^nA^{m+1}B_{p+1}) = A^p(A^{m+1}B_{p+1}) = O.
\]
By an application of the mathematical induction, we have
\[
A^nB_j = O \quad (n - 1 \leq j \leq p). \quad (4.12)
\]
Now, let \( \lambda = \infty \) and repeatedly using the fact that \( A \) and \( B_j \) commute, then from (3.4), (3.5) and (4.11) follows
\[
(\omega I + A)^{(m+1)n}A^n = (-1)^{m+1}[(\omega I - A)^{(m+1)n}]A^n
\]
\[
= (-1)^{m+1}[(\omega^n I + \lambda n^2 B_1 + \ldots + \lambda B_{n-1}) + B_{p+1})]p(\lambda)^{m+1}A^n
\]
\[
= (-1)^{m+1}A^n[\lambda B_{p+1}/a_p + \ldots + \lambda B_{p+1})/(\lambda^n + a\lambda^{n-2}B_1 + \ldots + a\lambda B_{p+1})]
\]
\[
= (-1)^{m+1}A^n(\lambda B_{p+1}/a_p + \ldots + a\lambda B_{p+1})]
\]
\[
= (-1)^{m+1}A^n(\lambda B_{p+1}/a_p + \ldots + a\lambda B_{p+1})]. \quad (4.12)
\]

Required result (4.9) follows from the last expression (4.12) and in the ref.\(^{18}\) by taking \( \lambda \to 0 \).

**Remark 4.4.** Since \( \text{Ind}(A) \leq n \), we can take \( m = n \) in (4.9). Smaller \( m \) is actually provided by the sequences \( \{a_j\} \) and \( \{B_j\} \) obtained from (3.7) and (3.8). Under the supposition of the Theorem 4.3, the algebraic multiplicity of the zero eigenvalue is \( n - p \). The fact \( n - p \geq \text{Ind}(A) \) of the Corollary 7.5.\(^{17}\) allows us to take \( m = n - p \) in the Theorem 4.3. Research of the sequences \( \{a_j\} \) and \( \{B_j\} \) shows that if \( \lambda \)
denotes the smallest integer such that \( B_\lambda = O \), then \( s - p \geq \text{Ind}(A) \). Thus, we can choose \( m = s - p \) in Theorem 4.3.

**Theorem 4.5.** Let \( A \in \mathbb{R}^{n \times n} \) with \( \text{Ind}(A) = i \). Then the general solution of the equation (4.4) is given by
\[
x = A^i(I - A^{i+1}u), \quad (4.13)
\]
where \( u \in \mathbb{R}^n \) is an arbitrary vector.

**Proof.** Let \( x = A^i(I - A^{i+1}u) \). Further it holds that
\[
Ax = AA^i(I - A^{i+1}u) = A(I - A^{i+1}u)u = (A - A^{i+1}A)u = (A - A^{i+1}u)u = Ou = 0.
\]

Conversely, assume that \( Ax = 0 \), then it holds that
\[
A^i(I - A^{i+1}u)(x_0 + u) = A^i(I - A^{i+1}u)x_0
\]
\[
= A^i(I - A^{i+1}u)A^i(u - x_0) + A^i(I - A^{i+1}A)x_0
\]
\[
= A^i(I - A^{i+1}u)(x - x_0) + A^i(I - A^{i+1}A)x_0.
\]

Thus, \( Ax = 0 = x = A^i(I - A^{i+1}u) \), for \( x = x_0 + u \).

**Remark 4.6.** For \( i = 1 \) and \( A^0 = A = B \), as a particular case of above theorem appears Theorem 1.1 earlier proved in the ref.\(^{140}\) or Theorem 17.1 proved in the ref.\(^{141}\) p. 174.

**Definition 4.7.** Chemical equation (4.1) is stable if \( \text{stab}(A) < 0 \).

**Lemma 4.8.** For any nonsingular matrix \( U \) and any vector norm \( |\cdot| \), with the induced \( \text{Lozinskii} \) measure \( \mu \), \( |Ux| \)
defines another vector norm and its induced matrix measure \( \mu_U \) is given by
\[
\mu_U(A) = \mu(UAU^T). \quad (4.14)
\]

**Proof.** The proof of this lemma follows directly from the Definition 3.12.

**Theorem 4.9.** For any matrix \( A \in \mathbb{R}^{n \times n} \) it holds
\[
\text{stab}(A) = \inf \{\mu(A), \mu \text{ is a Lozinskii measure on } \mathbb{R}^n\}. \quad (4.15)
\]

**Proof.** The relation (4.15) obviously holds for diagonalizable matrices in view of (4.14) and the first two relations in (3.12). Furthermore, the infimum in (4.15) can be achieved if the matrix \( A \) is diagonalizable. The general case can be shown based on this observation, the fact that \( A \) can be approximated by diagonalizable matrices in \( \mathbb{R} \) and the continuity of \( \mu(\cdot) \), which is implied by the property
\[
|\mu(3) - \mu(N)| \leq |3 - N|.
\]

**Remark 4.10.** From the above proof it follows that \( \text{stab}(A) = \inf \{\mu_u(UAU^T), \det U \neq 0\} \). The same relation holds if \( \mu_u \) is replaced by \( \mu_k \).

**Corollary 4.11.** Let \( A \in \mathbb{R} \). Then \( \text{stab}(A) < 0 \Leftrightarrow \mu(A) < 0 \) for some \( \text{Lozinskii} \) measure \( \mu \) on \( \mathbb{R}^n \).

More results for stability criteria are obtained in works.\(^{142,143}\)
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 known 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 chemical equation

\[
x_1 \text{MoI(NH}_3\text{)}_5\text{SO}_4 + x_2 \text{MgCl}_2 + x_3 \text{Mn}_2\text{O}_3 + x_4 \text{H}_3\text{PO}_4 + x_5 \text{KCl} = x_6 \text{K}_2\text{.98PO}_4 + x_7 \text{Mo(NH}_3\text{)}_6\text{Cl}_3 + x_8 \text{MgI}_2 + x_9 \text{H}_2\text{O} + x_{10} \text{N}_2\text{O}_3 + x_{11} \text{MnSO}_4. \tag{5.1}
\]

According to the scheme

\[
\begin{array}{ccccccccc}
\text{MoI(NH}_3\text{)}_5\text{SO}_4 & \text{MgCl}_2 & \text{Mn}_2\text{O}_3 & \text{H}_3\text{PO}_4 & \text{KCl} & \text{K}_2\text{.98PO}_4 & \text{Mo(NH}_3\text{)}_6\text{Cl}_3 & \text{MgI}_2 & \text{H}_2\text{O} & \text{N}_2\text{O}_3 & \text{MnSO}_4 \\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & 0 & 0 & -6 & 0 & 0 & -2 & 0 \\
15 & 0 & 0 & 3 & 0 & 0 & -18 & 0 & -2 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
4 & 0 & 3 & 4 & 0 & -4 & 0 & 0 & -1 & -3 & -4 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 1 & 0 & -3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & -2.98 & 0 & 0 & 0 & 0 & 0 \\
\end{array}
\]

the reaction matrix is

\[
A = \begin{bmatrix}
1 & 0 & 0 & 0 & 0.00 & -1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0.00 & 0 & -2 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & 0 & 0.00 & -6 & 0 & 0 & -2 & 0 & 0 \\
15 & 0 & 0 & 3 & 0.00 & -18 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0.00 & 0 & 0 & 0 & 0 & 0 & -1 \\
4 & 0 & 3 & 4 & 0.00 & -4.00 & 0 & 0 & 0 & -1 & -3 & -4 \\
0 & 1 & 0 & 0 & 0.00 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 1.00 & 0 & -3 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 0 & 0.00 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 1 & -1.00 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1.00 & -2.98 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}.
\]

The rank of the above matrix is \(r = 11\). Since the nullity of the reaction matrix is \(k = n - r = 11 - 11 = 0\), then we have only a trivial solution \(x = 0\), 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. Consider this equation

\[
x_1 \text{KAu(CN)}_4 + x_2 \text{KAu(CN)}_2\text{Cl}_2 + x_3 \text{KHCl}_2 + x_4 [\text{4Fe(CN)}_3\cdot3\text{Fe(CN)}_2]+ x_5 [\text{PtCl}_3\cdot7\text{H}_2\text{O}] = x_6 [\text{Pt(NH}_3\text{)}_2\cdot\text{C}_5\text{H}_4\text{ON})_2\cdot\text{NO}_3\cdot2\text{H}_2\text{O}] + x_7 \text{K}_3\text{.99Fe(CN)}_6 + x_8 \text{HAuCl}_3 + x_9 \text{NO}_2. \tag{5.2}
\]

According to the scheme

\[
\begin{bmatrix}
\text{KAu(CN)}_4 & \text{KAu(CN)}_2\text{Cl}_2 & \text{KHCl}_2 & [\text{4Fe(CN)}_3\cdot3\text{Fe(CN)}_2] & [\text{PtCl}_3\cdot7\text{H}_2\text{O}] & [\text{Pt(NH}_3\text{)}_2\cdot\text{C}_5\text{H}_4\text{ON})_2\cdot\text{NO}_3\cdot2\text{H}_2\text{O}] & \text{K}_3\text{.99Fe(CN)}_6 & \text{HAuCl}_3 & \text{NO}_2 \\
0 & 0 & 1 & 0 & 14 & -24 & 0 & -1 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 2 & 0 & 0 & 7 & 0 & 0 & -1 & 0 \\
4 & 2 & 0 & 18 & 0 & 0 & 0 & -6 & 0 \\
0 & 4 & 2 & 0 & 18 & 0 & -8 & -6 & 0 \\
0 & 0 & 0 & 0 & 7 & 0 & -10 & 0 & 0 \\
0 & 0 & 1 & 0 & 14 & 0 & 7.00 & 0 & -2 \\
0 & 0 & 0 & 0 & 10.00 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 10.00 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 10.00 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 7.00 & 10.00 & 0 & 2 & 0 \\
\end{bmatrix}.
\]
The rank of the above matrix is \( r = 8 \). Since the nullity of the reaction matrix is \( k = n - r = 9 - 8 = 1 \), then we have a non-trivial solution \( x \neq 0 \), that means that the reaction is feasible.

Since \( \text{rank} A = \text{rank} A^2 = 8 \), that means that \( \text{Ind}(A) = 1 \). In order to determine the group inverse \( A^\# \) of \( A \), we will use the recursive formulae (3.6)-(3.8) and Theorem 4.3. So, we obtain \( a_1 = -\text{tr} A = 15 \).

\[
B_1 = A + a_1 I =
\begin{bmatrix}
15.0 & 0.00 & 1.00 & 0.00 & 14.0 & -24.0 & 0.00 & -1.00 & 0.00 \\
1.00 & 16.0 & 0.00 & 0.00 & 0.00 & 0.00 & -1.00 & 0.00 & 0.00 \\
0.00 & 2.00 & 17.0 & 0.00 & 3.00 & 0.00 & 0.00 & -3.00 & 0.00 \\
1.00 & 1.00 & 15.0 & 0.00 & 0.00 & -3.99 & 0.00 & 0.00 & 0.00 \\
0.00 & 0.00 & 0.00 & 7.00 & 15.0 & 0.00 & -1.00 & 0.00 & 0.00 \\
4.00 & 2.00 & 0.00 & 18.0 & 0.00 & 5.00 & -6.00 & 0.00 & 0.00 \\
4.00 & 2.00 & 0.00 & 18.0 & 0.00 & -8.00 & 9.00 & 0.00 & -1.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 1.00 & -2.00 & 0.00 & 15.0 & 0.00 \\
0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 7.00 & -10.0 & 0.00 & 0.00 \\
\end{bmatrix}
\]

\[
AB_1 =
\begin{bmatrix}
-96.0 & -46.00 & 17.0 & -334.0 & 212.0 \\
16.0 & 16.0 & 1.00 & 0.00 & 13.00 \\
2.0 & 36.0 & 34.0 & 21.00 & 48.00 \\
0.04 & -10.02 & 18.0 & -71.82 & 17.00 \\
3.00 & 5.00 & 7.00 & 87.00 & 0.000 \\
16.0 & 18.00 & 22.00 & -18.00 & 56.00 \\
24.0 & 22.00 & 22.00 & 18.00 & 49.00 \\
-8.00 & -4.000 & 0.00 & -29.00 & 15.00 \\
-40.0 & -20.00 & 0.00 & -131.0 & 91.00 \\
\end{bmatrix}
\]

\[
AB_2 =
\begin{bmatrix}
-332.0 & -322.00 & -236.18 & 1700.0 & 926.48 \\
87.82 & 133.82 & 18.000 & -305.00 & 210.00 \\
69.00 & 450.64 & 410.64 & 390.00 & 556.46 \\
-13.940 & 78.040 & 124.04 & -384.82 & 77.490 \\
-23.720 & 48.140 & 104.00 & 598.00 & 70.000 \\
-16.00 & 36.000 & 42.000 & 320.00 & 326.00 \\
-56.00 & 92.000 & 86.000 & 415.00 & 347.00 \\
-29.00 & -31.000 & -37.000 & 123.00 & 47.820 \\
-59.00 & -105.00 & -171.00 & 1051.0 & 376.74 \\
\end{bmatrix}
\]

\[
a_1 = -(\text{tr} AB_2)/3 = 359.82, B_3 = AB_2 + a_1 I =
\begin{bmatrix}
27.82 & -322.00 & -236.18 & 1700.0 & 926.48 \\
87.82 & 493.64 & 18.000 & -305.00 & 210.00 \\
69.00 & 450.64 & 770.46 & 390.00 & 556.46 \\
-13.940 & 78.040 & 124.04 & -384.82 & 77.490 \\
-23.720 & 48.140 & 104.00 & 598.00 & 70.000 \\
-16.00 & 36.000 & 42.000 & 320.00 & 326.00 \\
-56.00 & 92.000 & 86.000 & 415.00 & 347.00 \\
-29.00 & -31.000 & -37.000 & 123.00 & 47.820 \\
-59.00 & -105.00 & -171.00 & 1051.0 & 376.74 \\
\end{bmatrix}
\]

\[
a_2 = -(\text{tr} AB_2)/2 = 159.82, B_4 = AB_2 + a_2 I =
\begin{bmatrix}
63.82 & 46.000 & 17.000 & -334.0 & 212.00 \\
16.00 & 175.82 & 1.000 & 0.000 & 13.000 \\
2.00 & 36.000 & 193.82 & 21.000 & 48.000 \\
0.04 & 10.020 & 18.000 & 88.000 & 17.000 \\
3.00 & 5.0000 & 7.0000 & 87.000 & 159.82 \\
16.00 & 18.000 & 22.000 & -18.000 & 56.000 \\
24.00 & 22.000 & 22.000 & 18.000 & 49.000 \\
-8.00 & -4.0000 & 0.0000 & -29.000 & 15.000 \\
-40.00 & -20.000 & 0.0000 & -131.0 & 91.000 \\
\end{bmatrix}
\]

\[
a_3 = -(\text{tr} AB_3)/3 = 359.82, B_5 = AB_4 + a_2 I =
\begin{bmatrix}
-118.00 & 130.0 & -18.000 & 0.0000 \\
-22.000 & 0.000 & -17.000 & 0.0000 \\
6.0000 & -3.000 & -53.000 & 0.0000 \\
7.9200 & -35.91 & -5.0000 & 3.9900 \\
8.0000 & -36.93 & 0.0000 & 1.0000 \\
61.820 & -65.82 & -6.0000 & 6.0000 \\
-78.000 & 82.00 & -6.0000 & -7.0000 \\
-10.000 & 11.00 & 159.82 & 0.0000 \\
-30.000 & 53.00 & 0.0000 & 133.82 \\
\end{bmatrix}
\]
\[ AB_1 = \]
\[
\begin{bmatrix}
149.92 & 291.600 & 1255.46 & 959.00 & -1297.88 \\
144.64 & 202.640 & -181.180 & 1272.0 & 1088.66 \\
329.48 & 2125.98 & 1999.92 & 1595.0 & 2678.92 \\
-38.800 & 255.200 & 209.140 & 129.15 & 308.410 \\
-153.58 & 454.280 & 782.280 & -590.00 & 195.430 \\
-140.00 & 192.000 & 388.000 & 50.00 & 178.740 \\
-113.00 & 369.000 & 643.000 & -361.00 & 454.000 \\
8.2800 & -23.8600 & 20.0000 & -42.0000 & -222.180 \\
111.96 & 186.980 & 650.000 & -116.0 & -1004.74 \\
\end{bmatrix}
\]
\[ = 5937.48 -5867.36 & 1002.72 & -788.66 \\
-1370.04 & 1072.95 & -635.460 & -119.00 \\
531.240 & -1345.82 & -2831.02 & 143.79 \\
12.6200 & 160.020 & -436.220 & 144.32 \\
1610.54 & -1616.26 & -336.420 & 263.51 \\
1365.44 & -858.800 & -146.000 & -147.46 \\
154.00 & -1072.85 & 406.000 & 288.7900 \\
461.080 & -413.010 & 171.000 & -72.710 \\
357.68 & -3319.17 & 677.000 & -372.05 \\
\]

\[ a_1 = -\frac{\text{tr}(AB_1)}{4} = -692.15, \quad B_1 = AB_1 + a_1J = \]
\[ \begin{bmatrix}
-542.23 & 291.600 & 1255.46 & 959.00 & -1297.88 \\
144.64 & -489.510 & -181.180 & 1272.0 & 1088.66 \\
329.48 & 2125.98 & 1999.92 & 1595.0 & 2678.92 \\
-38.800 & 255.200 & 209.140 & 129.15 & 308.410 \\
-153.58 & 454.280 & 782.280 & -590.00 & 195.430 \\
-140.00 & 192.000 & 388.000 & 50.00 & 178.740 \\
-113.00 & 369.000 & 643.000 & -361.00 & 454.000 \\
8.2800 & -23.8600 & 20.0000 & -42.0000 & -222.180 \\
111.96 & 186.980 & 650.000 & -116.0 & -1004.74 \\
\end{bmatrix} \]

\[ AB_2, AB_3, AB_4 = \]
\[ \begin{bmatrix}
10116.8 & 8953.2 & 5610.9 & 4772.0 & 6373.7 \\
-4175.60 & 1517.0 & 3975.7 & 4860.0 & 7475.6 \\
-741.480 & 2759.2 & 3283.9 & 4056.0 & 5603.0 \\
-27.4400 & 106.88 & 107.72 & 2019.3 & 823.64 \\
2571.32 & 2346.3 & 2096.6 & 1516.0 & 5219.7 \\
1857.10 & 1580.0 & -1216.0 & 1022.0 & 1917.5 \\
756.000 & 1988.0 & -1400.0 & -756.0 & 1224.0 \\
841.480 & 123.44 & 551.02 & 596.0 & 478.92 \\
3688.16 & 1680.0 & -1705.1 & 616.0 & 1965.5 \\
\end{bmatrix} \]

\[ \begin{bmatrix}
1531.08 & 3901.76 & 2927.69 & -7823.00 & -8342.74 \\
-405.870 & -174.050 & 1054.28 & 2273.00 & 12.9600 \\
462.660 & 4707.36 & 4540.02 & 4090.0 & 6711.54 \\
382.760 & 455.760 & -183.520 & 5266.39 & 658.240 \\
-158.600 & 1417.40 & 820.980 & -3580.0 & 1704.87 \\
-500.040 & 646.980 & 686.000 & -2088.00 & -1974.22 \\
-892.000 & 844.000 & 812.000 & -872.000 & -612.000 \\
126.420 & 70.2800 & 6.28000 & -690.000 & -854.200 \\
101.020 & 886.000 & 295.960 & -2398.00 & -3254.96 \\
\end{bmatrix} \]

\[ \begin{bmatrix}
6458.76 & -2949.25 & -3515.75 & 7444.68 \\
4106.36 & -4381.40 & 888.410 & -834.950 \\
1770.78 & -4155.49 & -6378.77 & 1058.24 \\
-1045.92 & 902.120 & -843.820 & -448.660 \\
-1451.66 & 2885.14 & -2647.54 & 1089.24 \\
5264.10 & 734.820 & -1216.00 & 1153.72 \\
3034.00 & 2336.39 & -2185.00 & 1923.00 \\
263.960 & 101.340 & -44.4200 & 558.430 \\
-2612.48 & 3912.52 & -2248.94 & 5447.57 \\
\end{bmatrix} \]

\[ \begin{bmatrix}
-3643.31 & 3901.76 & 2927.69 & -7823.00 & -8342.74 \\
-405.870 & -5348.44 & 1054.28 & 2273.00 & 12.9600 \\
462.660 & 4707.36 & -6343.70 & 4090.00 & 6711.54 \\
382.760 & 455.760 & -183.520 & 820.980 & -3580.00 & -1974.22 \\
-158.600 & 1417.40 & 820.980 & -3580.0 & 1704.87 \\
-500.040 & 646.980 & 686.000 & -2088.00 & -1974.22 \\
-892.000 & 844.000 & 812.000 & -872.000 & -612.000 \\
126.420 & 70.2800 & 6.28000 & -690.000 & -854.200 \\
101.020 & 886.000 & 295.960 & -2398.00 & -3254.96 \\
\end{bmatrix} \]
\[ a_0 = -\frac{(\text{tr}AB_6)}{6} = -\frac{2247.28}{6}, B_6 = AB_5 + a_0I = \]
\[
\begin{bmatrix}
7869.5 & 8953.2 & -5610.9 & 4772.0 & 6373.7 \\
-4175.6 & -3764.2 & 3975.7 & -4860.0 & -7475.6 \\
-741.48 & 2759.2 & 1036.6 & 4056.0 & 5603.0 \\
-27.440 & -106.88 & 107.72 & -228.00 & 823.64 \\
3571.3 & 2346.3 & -2096.6 & 1516.0 & 2972.4 \\
1857.1 & 1580.0 & -1216.0 & 1022.0 & 1917.5 \\
756.0 & 1988.0 & -1400.0 & -756.0 & 1224.0 \\
841.48 & 123.44 & -551.02 & 596.0 & 478.92 \\
3688.2 & 1680.0 & -1705.1 & 616.0 & 1965.5 \\
\end{bmatrix}
\]

\[ a_9 = -(\text{tr}AB_8)/9 = 0, B_9 = AB_8 + a_9I = \]
\[
\begin{bmatrix}
-20969.5 & 18499.4 & -9041.52 & -11940.11 \\
10301.2 & -7431.99 & 2591.47 & 6051.300 \\
6607.42 & -8722.38 & -3266.91 & 2039.01 \\
238.8 & -162.52 & -287.96 & 4800000 \\
1035.94 & 9152.84 & -3721.74 & -5063.620 \\
1267.18 & 5358.16 & -2204.94 & -3042.260 \\
1088.00 & 668.00 & -2388.00 & -1008.00 \\
1631.08 & 1415.50 & -2462.82 & -1218.200 \\
5833.76 & 5022.74 & -1874.90 & -6706.160 \\
\end{bmatrix}
\]

\[ AB_6 = \]
\[
\begin{bmatrix}
3845.12 & -2246.72 & 1419.7 & 156.00 & 718.200 \\
2852.44 & 565.48 & 1084.2 & -684.00 & -1580.76 \\
-1644.64 & 4568.56 & 5387.8 & 1152.00 & 3735.36 \\
-64.0000 & 16.0000 & -40.0000 & 6984.44 & -382.560 \\
-948.080 & -2736.16 & 894.04 & -840.00 & 4541.48 \\
-474.040 & -1368.08 & 447.02 & -420.00 & -1149.48 \\
-448.000 & 112.000 & -280.00 & 1008.00 & 720.000 \\
-142.880 & -813.760 & 353.44 & -528.00 & -862.560 \\
-948.080 & -2736.16 & 894.04 & -840.00 & -2298.96 \\
\end{bmatrix}
\]

\[ a_8 = -\frac{(\text{tr}AB_8)}{8} = 3397.92, B_8 = AB_7 + a_8I = \]
\[
\begin{bmatrix}
10314.7 & -10592.96 & 10.1100 & 5380.77 \\
-9037.22 & 9651.960 & -3987.23 & -6706.61 \\
7644.08 & -9096.720 & -5127.64 & 4644.36 \\
280.240 & -320.2400 & 188.840 & 172.120 \\
2699.68 & -1805.640 & 372.280 & 974.400 \\
8686.60 & -1381.140 & 210.980 & 726.360 \\
2248.00 & 4312.440 & -2324.00 & 1348.00 \\
1898.92 & -1563.480 & 688.140 & 1020.90 \\
451.240 & 442.8000 & -252.980 & 8389.58 \\
\end{bmatrix}
\]

\[ a_7 = -\frac{(\text{tr}AB_7)}{7} = 6840.44, B_7 = AB_6 + a_7I = \]
\[
\begin{bmatrix}
-2995.3 & -2436.72 & 1419.7 & 156.00 & 718.200 \\
2852.4 & -1774.96 & -1084.2 & -684.00 & -1580.76 \\
-1644.6 & 4658.56 & -1452.6 & 1152.0 & 3735.36 \\
-64.0000 & 16.0000 & 40.0000 & 1440.00 & -382.560 \\
-948.08 & -2736.16 & 894.04 & -840.00 & -2298.96 \\
-474.04 & -1368.08 & 447.02 & -420.00 & -1149.48 \\
-448.00 & 112.00 & -280.00 & 1008.00 & 720.000 \\
142.88 & 813.760 & 353.44 & -528.00 & -862.560 \\
-948.08 & -2736.16 & 894.04 & -840.00 & -2298.96 \\
\end{bmatrix}
\]

\[ AB_7 = \]
\[
\begin{bmatrix}
-3397.92 & 0.0000 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & -3397.92 & 0.0000 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & -3397.92 & 0.0000 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & -3397.92 & 0.0000 \\
0.0000 & 0.0000 & 0.0000 & 0.0000 & -3397.92 \\
\end{bmatrix}
\]

\[ a_6 = -\frac{(\text{tr}AB_6)}{6} = -\frac{2247.28}{6}, B_6 = AB_5 + a_0I = \]
\[
\begin{bmatrix}
10314.66 & -10593.96 & 10.1100 & 5380.77 \\
-9037.22 & 9651.960 & -3987.23 & -4670.61 \\
7644.080 & -9096.720 & -5127.64 & 4644.36 \\
280.240 & -320.2400 & 188.840 & 172.120 \\
2699.680 & -1805.640 & 372.280 & 974.400 \\
8686.60 & -1381.140 & 210.980 & 726.360 \\
2248.00 & 4312.440 & -2324.00 & 1348.00 \\
1898.92 & -1563.480 & 688.140 & 1020.90 \\
451.240 & 442.8000 & -252.980 & 8389.58 \\
\end{bmatrix}
\]

Since \( m = s - p = 9 - 8 = 1 \), according to (4.9) and Definition 3.3, the group inverse \( A^* \) of \( A \), obtains this form

\[ A^* = (AB_7)^2/(a_6)^2 = (3397.92)^2 \times \]

\[ AB_4 = O, \text{tr}(AB_4) = 0, a_0 = -\frac{(\text{tr}AB_8)}{9} = 0, B_9 = AB_8 + a_9I = O. \]
while required vector is

\[ x = (I - A^T A)^{-1} u = \begin{bmatrix} 0.29591043932758864246 \\ 0.54870038140980364458 \\ 0.33903093657296228281 \\ 0.04237886707162028535 \\ 0.25278994208221500212 \end{bmatrix} \]

where \( u^T = (1, 1, 1, 1, 1, 1, 1, 1, 1) \) was employed as an arbitrary vector.

Therefore, balanced chemical equation (5.2) looks like this

\[
\begin{align*}
0.29591043932758864246\text{KAu(CN)}_4 &+ 0.54870038140980364458\text{KAu(CN)}_2\text{Cl}_2 \\
0.33903093657296228281\text{KCl} &+ 0.04237886707162028535[4\text{Fe(CN)}_3\cdot3\text{Fe(CN)}_2] \\
0.25278994208221500212[\text{PtCl}_3\cdot7\text{H}_2\text{O}] &
\end{align*}
\]

and

\[
0.12639497104110750106 \times \left[ \text{Pt(NH}_3)_2(C_3\text{H}_4\text{ON})_2\right]\text{(NO}_3)_2\cdot2\text{H}_2\text{O} \\
+ 0.29665206950134199745\text{K}_{1.99}\text{Fe(CN)}_6 \\
+ 0.84461082073739228704\text{HauCl}_3 \\
+ 0.25278994208221500212\text{NO}_2
\]

If we multiply the above equality by 9438.6666666666666667 we obtain

\[
2793\text{KAu(CN)}_4 + 5179\text{KAu(CN)}_2\text{Cl}_2 + 3200\text{KCl}_2 \\
+ 400[4\text{Fe(CN)}_3\cdot3\text{Fe(CN)}_2] + 2386[\text{PtCl}_3\cdot7\text{H}_2\text{O}] \\
= 1193[\text{Pt(NH}_3)_2(C_3\text{H}_4\text{ON})_2]\text{(NO}_3)_2\cdot2\text{H}_2\text{O} \\
+ 2800\text{K}_{1.99}\text{Fe(CN)}_6 \\
+ 7972\text{HauCl}_3 + 2386\text{NO}_2
\]

The eigenvalues of the matrix \((A + A^T)/2\) are

\[
\begin{align*}
\lambda_1 &= -24.0794746107446, \\
\lambda_2 &= -11.2916856690336, \\
\lambda_3 &= 12.1067307988895, \\
\lambda_4 &= 7.73871001726729, \\
\lambda_5 &= 3.0200573473832, \\
\lambda_6 &= -2.2722437433717, \\
\lambda_7 &= 1.01502554923706, \\
\lambda_8 &= -0.246450556871925, \\
\lambda_9 &= -0.99660024870706.
\end{align*}
\]

The Lozinskii measures of \(A\) given by (3.12) with respect to the three common norms (3.11) are

\[
\begin{align*}
\mu_1(A) &= \max (40, 3, 10, 6.99, 8, 20, 27, 3, 15) = 40, \\
\mu_2(A) &= \max (10, 8, 4, 43, 25, 34, 4.99, 5, -1) = 43, \\
\mu_3(A) &= \lambda_3 = 12.1067307988895.
\end{align*}
\]

Since \(\mu_2(A) > 0\) and definition 4.7 immediately follows that the chemical equation (5.2) is unstable.

With this method we balanced successfully lot of chemical equations and some of them are given below as examples. The research shown that considered chemical equations are unstable too.

**Example 5.3.**

\[
\begin{align*}
255650\text{AgO} \cdot [\text{Ru(C}_10\text{H}_8\text{N}_2)_3]\text{Cl}_2\cdot6\text{H}_2\text{O} \\
+ 7937524\text{CsMn(CN)}_6 \\
+ 1700898\text{C}_2\text{H}_5\text{AuNaOS}_7 + 3128756\text{H}_2\text{CO}_3 \\
+ 1515242\text{Au}_2\text{O} + 14341148\text{NO}_2 + 2040087\text{TeO}_3 \\
= 255650\text{Pt(NH}_3)_2\cdot\text{ClNO}_3 + 3968762\text{Mn}_2(\text{SO}_4)_3 \\
+ 31750096\text{K}_{1.97}\text{Au(CN)}_2 + 1726800\text{Na}_{1.97}\text{CO}_3 + 511300\text{HCl} \\
+ 10026153\text{H}_2\text{O} \\
(5.3)
\end{align*}
\]

**Example 5.4.**

\[
\begin{align*}
152208\text{AgAuPtTe}_6\cdot[(\text{NH}_3)\text{HClO}_3] \\
+ 131202\text{Cu}_3\text{H}_5\text{AuNaOS}_7 + 612276\text{K}_{1.97}\text{Fe(CN)}_6 \\
+ 69412\text{Ru}(\text{CO})_6 \\
+ 108287\text{Au}_2\text{O} + 1376760\text{HNO}_3 \\
+ 152208\text{Pt(NH}_3)_2\text{ClNO}_3 + 133200\text{Na}_{1.97}\text{CO}_3 \\
+ 2449104\text{Au(CN)}_2 + 306138\text{Fe}_2(\text{SO}_4)_3 \\
+ 208236\text{RuO}_2 + 913248\text{TeO}_3
\end{align*}
\]
Example 5.5.
\[47886 \text{NH}_4\text{ClO}_4 + 84000 \text{NaLa(OH)}_4 + 207C_55H_72\text{CdN}_4\text{O}_5 + 588[\text{WCl}_4(\text{NSeCl})_2] + 26805\text{HNO}_3 + 16332180\text{H}_2\text{CO}_3 + 4620\text{CuCoO}_4 + 9273600\text{W}_2\text{O} + 36960\text{SO}_2. \quad (5.4)\]

Example 5.6.
\[47886 \text{NH}_4\text{ClO}_4 + 84000 \text{NaLa(OH)}_4 + 207C_55H_72\text{CdN}_4\text{O}_5 + 588[\text{WCl}_4(\text{NSeCl})_2] + 26805\text{HNO}_3 + 16332180\text{H}_2\text{CO}_3 + 4620\text{CuCoO}_4 + 9273600\text{W}_2\text{O} + 36960\text{SO}_2. \quad (5.4)\]

Example 5.7.
\[1248C_6\text{H}_7\text{MgN}_4\text{O}_5 + 588[\text{WCl}_4(\text{NSeCl})_2] + 26805\text{HNO}_3 + 16332180\text{H}_2\text{CO}_3 + 4620\text{CuCoO}_4 + 9273600\text{W}_2\text{O} + 36960\text{SO}_2. \quad (5.4)\]

Example 5.8.
\[97776C_44H_32\text{BrN}_2\text{O}_2\text{P}_2 + 25596C_44H_32F_5\text{NP}_2\text{Pt} + 1502160[\text{Ru}(\text{Cl}_6\text{H}_2\text{N}_2)_3]\text{Cl}_2 + 1698748\text{H}_2\text{CO}_3 + 4620\text{CuCoO}_4 + 9273600\text{W}_2\text{O} + 36960\text{SO}_2. \quad (5.4)\]
will solve more two chemical equations, which remain in chemistry to date as open problems.

**Example 5.11.** As an unbalanced equation Jensen in the ref.144 proposed this equation

\[
x_1 \text{NH}_4\text{ClO}_4 + x_2 \text{HNO}_3 + x_3 \text{HCl} + x_4 \text{H}_2\text{O} = x_5 \text{ClO}_4\text{2H}_2\text{O} + x_6 \text{N}_2\text{O}_5 + x_7 \text{NO} + x_8 \text{NO}_2 + x_9 \text{Cl}_2.
\]

(5.11)

Actually, it was not a new chemical equation, but it represents only a slight modification of the well-known Willard’s equation considered long time ago.145 Also, the above equation was considered from Weltin,25 but unfortunately he did not offer its solution. It is good to emphasize that Jensen144 states that this equation has no single unique lowest whole numbers solution. This Jansen’s statement we will refute here, because it is wrong.

Here we will determine the general solution of (5.11) as well as its minimal solution according to the Jensen’s requirements. First we will determine its general solution. From the above chemical equation follows this system of linear equations

\[
\begin{align*}
    x_1 + x_2 &= 2x_6 + x_7 + x_8, \\
    4x_1 + x_2 + x_3 + 2x_4 &= 5x_5, \\
    x_1 + x_3 &= x_5 + 2x_9, \\
    4x_1 + 3x_2 + x_3 &= 6x_1 + x_6 + x_7 + 2x_8.
\end{align*}
\]

The general solution of this system is

\[
\begin{align*}
    x_5 &= -\frac{4x_1}{5} + x_2/5 + x_3/5 + 2x_4/5, \\
    x_7 &= -(14x_1)/5 + x_2/5 + 6x_3/5 + 7x_4/5 + 3x_6, \\
    x_8 &= 9x_1/5 - 4x_2/5 + 6x_3/5 + 7x_4/5 + x_6, \\
    x_9 &= -x_1/10 + x_2/10 - 2x_3/5 + x_4/5, \\
\end{align*}
\]

where \(x_1, x_2, x_3, x_4\) and \(x_6\) are arbitrary real numbers.

Now, the balanced equation has a form

\[
x_1 \text{NH}_4\text{ClO}_4 + x_2 \text{HNO}_3 + x_3 \text{HCl} + x_4 \text{H}_2\text{O} = -(4x_1/5 + x_2/5 + x_3/5 + 2x_4/5) \text{ClO}_4\text{2H}_2\text{O} \\
+ x_6 \text{N}_2\text{O}_5 - (14x_1/5 + x_2/5 + 6x_3/5 + 7x_4/5 + 3x_6) \text{NO} \\
+ (9x_1/5 - 4x_2/5 + 6x_3/5 + 7x_4/5 + x_6) \text{NO}_2 \\
+ (-x_1/10 + x_2/10 - 2x_3/5 + x_4/5) \text{Cl}_2,
\]

where \(x_1, x_2, x_3, x_4\) and \(x_6\) are arbitrary real numbers.

This is okay from a mathematical view point. It means that the reaction (5.11) has infinity number modifications, but in chemistry it is important to be determined the unique minimal coefficients \(x_i\in\mathbb{R}\) (1 ≤ \(i\) ≤ 9).

For that purpose we will use the newest pseudo-inverse matrix method for balancing chemical equations given in the ref.9 According to the theorem 4.2,9 the equation (5.11) reduces to a Diophantine matrix equation

\[
Ax = By,
\]

where

\[
A = \begin{bmatrix} 1 & 0 & 0 \\ 4 & 1 & 1 \\ 1 & 0 & 1 \\ 4 & 3 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 2 & 1 & 1 & 0 \\ 5 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 2 \\ 6 & 1 & 1 & 2 \end{bmatrix},
\]

\(x^\top = (x_1, x_2, x_3, x_4)\) and \(y^\top = (x_5, x_6, x_7, x_8, x_9)\) are required vectors and \(T\) denotes transpose.

From the theorem 4.39 follows that the general solution of the Diophantine matrix equation is given by

\[
y = (I - GG)u = \begin{bmatrix} 0.0332 \\ -0.0184 \\ 0.2546 \\ -0.2180 \\ 0.0665 \end{bmatrix},
\]

and

\[
x = A^\top By + (I - A^\top A)v = \begin{bmatrix} -0.4585 \\ 0.4583 \\ 0.6247 \\ 0.4585 \end{bmatrix},
\]

where

\[
G = (I - AA^\top)B,
\]

\[
A^\top = \begin{bmatrix} 0.024193548387 & 0.104838709677 & 0.169354838710 -0.266429032258 \\ 0.137096774194 -0.072580645161 & -0.282258064516 & 0.443548387097 \\ 0.145161290323 & 0.040322580645 & 0.016129032258 & 0.282258064516 \\ 0.822580645161 -0.104838709677 & -0.693548387097 -0.137096774194 \end{bmatrix}
\]

is the Moore-Penrose pseudoinverse matrix of \(A, u^\top = (1, 1, 1, 1, 1)\) and \(v^\top = (1, 1, 1, 1, 1)\).

This solution is unique, because is unique the Moore-Penrose pseudoinverse matrix \(A^\top\).

Now, balanced equation (5.11) with minimal coefficients will has this form

\[\text{Ax} = \text{By},\]
A New Singular Matrix Method

- 0.4585 NH₄ClO₄ + 0.4583 HNO₃ + 0.6247 HCl + 0.4585 H₂O = 0.0332 HClO₂ + 0.0184 N₂O + 0.2546 NO – 0.2180 NO₂ + 0.0685 Cl₂,

or in a conventional form

4583 HNO₃ + 6247 HCl + 4585 H₂O + 2180 NO₂ + 184 N₂O = 4585 NH₄ClO₄ + 332 HClO₂ + 2H₂O + 2546 NO + 665 Cl₂.

By this the problem is completely solved.

Example 5.12. Melville⁴³ proposed this chemical equation

\[ x_1 \text{KNO}_3 + x_2 \text{C} + x_3 \text{S} = x_4 \text{K}_2\text{CO}_3 + x_5 \text{K}_2\text{SO}_4 + x_6 \text{K}_2\text{S}_2 + x_7 \text{CO}_2 + x_8 \text{CO} + x_9 \text{N}_2. \] (5.12)

From the above chemical equation follows this system of linear equations

\[
\begin{align*}
x_1 &= 2x_4 + 2x_5 + 2x_6, \\
x_2 &= 2x_5, \quad 3x_1 = 3x_4 + 4x_5 + 2x_7 + x_8, \\
x_2 &= 4x_7 + x_8 + x_9, \\
x_3 &= x_5 + 2x_6,
\end{align*}
\]

which general solution is

\[
\begin{align*}
x_3 &= x_1 - x_3 - 2x_4, \quad x_6 = -x_1/2 + x_3 + x_4, \\
x_7 &= -x_1 - x_2 + 4x_3 + 6x_4, \\
x_9 &= x_1 + 2x_2 - 4x_3 - 7x_4, \quad x_9 = x_5/2, \\
\end{align*}
\]

where arbitrary numbers \(x_i \in \mathbb{R} (1 \leq i \leq 4).\)

Now, the balanced equation has a form

\[
\begin{align*}
x_1 \text{KNO}_3 + x_2 \text{C} + x_3 \text{S} &= x_4 \text{K}_2\text{CO}_3 + (x_1 - x_3 - 2x_4) \text{K}_2\text{SO}_4 \\
&+ (-x_1/2 + x_3 + x_4) \text{K}_2\text{S}_2 + ((-x_1 - x_2 + 4x_3 + 6x_4) \text{CO}_2 \\
&+ (x_1 + 2x_2 - 4x_3 - 7x_4) \text{CO} + x_5/2 \text{N}_2,
\end{align*}
\]

where arbitrary numbers \(x_i \in \mathbb{R} (1 \leq i \leq 4).\)

The minimal solution we determined with the same procedure as in the previous example, such that balanced equation (5.12) with minimal coefficients has this form

\[
\begin{align*}
x_1 &= 0.3700 \text{KNO}_3 + 1.9768 \text{CO} + 0.2783 \text{S}, \\
&= 0.3327 \text{K}_2\text{CO}_3 - 0.5737 \text{K}_2\text{SO}_4 \\
&+ 0.4260 \text{K}_2\text{S}_2 + 0.7626 \text{CO}_2 \\
&+ 0.8815 \text{CO} + 0.1850 \text{N}_2,
\end{align*}
\]

or in its conventional form it looks like this

\[
\begin{align*}
3700 \text{KNO}_3 + 5737 \text{K}_2\text{SO}_4 + 19768 \text{C} + 2783 \text{S} &= 3327 \text{K}_2\text{CO}_3 + 4260 \text{K}_2\text{S}_2 + 7626 \text{CO}_2 \\
&+ 8815 \text{CO} + 1850 \text{N}_2.
\end{align*}
\]

By this the required solution is completed.

Remark 5.12. This work and previous published works⁷⁹ make a circled scientific whole. Actually, by these works is completely solved century old problem of balancing chemical equations in its general form by using of generalized matrix inverses. Accurately speaking, it means that the general problem of balancing chemical equations from now remains behind us only like a history.

6. CONCLUSION

The practical superiority 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 possess fractional oxidation numbers. Research shown that employed singular matrix method founded by virtue of the Drazin pseudoinverse matrix works perfectly for the chemical equations which may be reduced to square matrix equation.

Actually, this method is unique method both in mathematics and chemistry which balances chemical equations with atoms which possess fractional as well as integer oxidation numbers, while all to date known methods for balancing chemical equations give an opportunity to balance chemical equations only with atoms which possess integer oxidation numbers. This is the main advantage of the method in relation of other known methods.

In other words, the mathematical method given here is applicable for all possible cases for balancing chemical equations, does not matter what kind of atoms they possess - fractional or integer oxidation numbers.

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 Lozinskii measures of the reaction matrix.

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REFERENCES
