

BALANCING CHEMICAL EQUATIONS USING RANK AND SOLVABILITY THEOREM

R. O. Akinola and U. P. Onyeulor

Department of Mathematics, Faculty of Natural Sciences, University of Jos, Nigeria

Abstract

A lot of work has been done on balancing Chemical equations. In this article, we show that (wx)maxima a free/cloned version of Maple can be used in balancing the most complex chemical reaction. In addition, we applied the Rank and Solvability theorem to tell whether or not the system of linear equations obtained from the chemical reaction is feasible in which case we either continue to balance the equation or conclude it is not feasible as the case may be. The work here is an improvement on the works of Hamid, which uses brute force to draw conclusions and it is time consuming.

1. Introduction

According to Risteski [1] a chemical reaction is an expression showing a symbolic representation of the reactants and products that is usually positioned on the left and right hand sides of a particular chemical reaction. Substances that takes part in a chemical reaction are represented by their molecular formula and their symbolic representation is also regarded as a chemical reaction [2]. A chemical reaction can either be reversible or irreversible. A chemical reaction, when it is feasible, is a natural process, the consequent equation is always consistent. Therefore, we must have non-trivial solutions and we should be able to obtain its assuming existences. Such an assumption is absolutely valid and does not introduce any error. If the reaction is infeasible, then there exists only the trivial solution, i.e., all coefficients are equal to zero [3].

These differs from Mathematical equations in the sense that while a single arrow (in the case of an irreversible reaction) or a double arrow points in the forward and backward directions of both the reactants and products (in the case of a reversible reaction) connects chemical reactions [4], an equality sign links the left and right hand sides of a Mathematical equation. 'The quantitative and qualitative knowledge of the chemical processes which estimates the amount of reactants, predicting the nature and amount of products and determining conditions under which a reaction takes place is important in balancing a chemical reaction. Balancing Chemical reactions is an excellent demonstrative and instructive example of the inter-connectedness between Linear Algebra and Stoichiometric principles' [3]. If the number of atoms of each type of element on the left is the same as the number of atoms of the corresponding type on the right, then the chemical equation is said to be balanced [4], otherwise it is not.

The qualitative study of the relationship between reactants in a chemical reaction is termed Stoichiometry [5]. Tuckerman [6] mentioned two methods for balancing a Chemical reaction: by inspection and algebraic.

The balancing-by-inspection method involves making successive intelligent guesses at making the coefficients that will balance an equation equal and continuing until the equation is balanced [3]. For simple equations this procedure is straight forward. However, according to [7], there is need for a 'step-by-step' approach which is easily applicable and can be mastered; rather than the haphazard hoping of inspection or a highly refined inspection. In addition, balancing-by-inspection method makes one to believe that there is only one possible solution rather than an infinite number of solutions which the method proposed in this paper illustrates. The algebraic approach circumvents the above loopholes provided in the inspection method and can handle complex chemical reactions.

The algebraic approach discussed in [6], involves putting unknown coefficients in front of each molecular species in the equation and solving for the unknowns. This is then followed by writing down the balance conditions on each element. After which he lets one of the unknowns to be one and takes turns to obtain the coefficients of the remaining unknowns. In the proposed approach, instead of setting one of the unknowns to zero, we write out the set of equations in matrix form, obtain a homogeneous system of equations. Since the system of equations is homogeneous, the solution obtained is in the nullspace of the corresponding matrix. This approach surpasses those in [3]; in the sense that we do not need to manually reduce the matrix to row reduced echelon form as shown in that paper. In their paper, they showed how the corresponding matrix is reduced to echelon form but did not use elementary row operations to convert it to row reduced echelon form. Akinola et al [8] used Matlab/octave rref command in balancing chemical equations. However, that command only gives the row reduced echelon form as floats instead of fractions.

Hamid [9] used brute force in balancing one of the most complex chemical reactions and also opined that Computer should not be used for such. In a most recent study by Candelario-Aplaon [10], she showed with the aid of Gauss-Jordan elimination and a free-online Matrix Calculator how to balance chemical equations. In fairness to the author, the Matrix Calculator gave the desired results without computing the row reduced echelon form as in our case where (wx)maxima's rref command was used. There were notational inconsistencies in [10] and there is no way to know if a chemical reaction is not feasible as we show.

In this article, we apply the Rank and Solvability theorem to analyze the balancing of chemical reactions. The use of this theorem circumvents the conclusions made by Hamid on the in feasibility of a certain chemical reaction. We also use the rref command in (wx)maxima which makes it easy in balancing even the most difficult chemical reaction with given reactants and products.

Corresponding Author: Akinola R.O., Email: roakinola@gmail.com, Tel: +2348185737399

Solved problems are provided to show that this methodology lends well for both simple and complex reactions. This is an improvement on an earlier work by Akinola et al [8], Gabriel et al [3] and circumvents the work of Hamid [9].

2. Methodology

In this section, we give the Rank and Solvability theorem and how it applies to determining the feasibility of a system resulting from a chemical equation. We also present the (wx)maxima code for finding the rref of a matrix. For complex equations, the most interesting thing is that (wx)maxima gives the rref in fractional form as will be shown on the examples in the next section.

Theorem 2.1. Rank and Solvability Theorem

Consider the system of equations $Ax = b$. Exactly one of the following three possibilities must hold.

1. The rank of the augmented matrix $[A|b]$ is greater than that of A and no solution exists to $Ax = b$.
2. The rank of the augmented matrix $[A|b]$ equals that of A , which equals the number of unknowns and the system $Ax = b$ has exactly one solution.
3. The rank of the augmented matrix $[A|b]$ equals that of A which is strictly less than the number of unknowns and the system $Ax = b$ has infinitely many solutions.

Proof: See [11].

Next, we give the definition of the rref command in (wx)maxima, which is the main tool of this paper.

This can be found in [12]

INPUT:

```
(%i1) rref(A) := block([p, q, k], [p, q] : matrix size(A), A : echelon(A),
k : min(p, q),
for i thru min(p, q) do (if A[i, i] = 0 then (k: i-1, return())),
for i : k thru 2 step -1 do (for j from i-1 thru 1 step -1 do A : rowop(A, j, i, A[j, i])),
A)$
```

The user needs not be an expert to use (wx) maxima.

3. Computational Examples

In this Section, we balance some chemical reactions by systems of linear equations. We begin by comparing the number of atoms of the reactants and the number of atoms of the product side to obtain the homogeneous system of equation. The most important fact to note in the context of this work is that the Rank and Solvability Theorems was used as a sufficient condition to conclude whether or not these chemical equations were balance-able. Since the resultant linear system of equations is homogeneous, we mostly perform row operations on the augmented matrix $[A|b] = [A|0]$, where 0 is the corresponding zero vector.

3.1 Example

Consider a chemical reaction [9]



In balancing the equation, let u, v, w, x, y and z be the unknown variables such that



Next, we compare the number of Potassium(K), Iron(Fe), Carbon(C), Nitrogen(N), Sulphur(S) and Oxygen(O) atoms of the reactants with the number of atoms of the product. We obtain six(6) linear equations:

$$K : 4u + 2v = 2x$$

$$Fe : u = z$$

$$C : 6u = w$$

$$N : 6u = y$$

$$S : 2v = x + z$$

$$O : 3v = 2w + 4x + 2y.$$

Rewriting these equations in standard form, we see a homogeneous linear system of equations in six unknowns;

$$4u + 2v - 2x = 0$$

$$u - z = 0$$

$$6u - w = 0$$

$$6u - y = 0$$

$$2v - x - z = 0$$

$$3v - 2w - 4x - 2y = 0.$$

The homogeneous system of equation becomes;

$$\begin{bmatrix} 4 & 2 & 0 & -2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 6 & 0 & -1 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ 0 & 3 & -2 & -4 & -2 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

where

$$A = \begin{bmatrix} 4 & 2 & 0 & -2 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & -1 \\ 6 & 0 & -1 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & -1 & 0 \\ 0 & 2 & 0 & -1 & 0 & -1 \\ 0 & 3 & -2 & -4 & -2 & 0 \end{bmatrix}, \quad x = \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix}, \quad \text{and} \quad b = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

INPUT:

(%i2) A: matrix([4,2,0,-2,0,0], [1,0,0,0,0,-1], [6,0,-1,0,0,0], [6,0,0,0,-1,0], [0,2,0,-1,0,-1], [0,3,-2,-4,-2,0]);

INPUT:

(%i3) rref(A);

Using wxmaxima, we obtained the rref A

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

The new augmented matrix becomes,

$$[A|b] = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & | & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & | & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & | & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & | & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & | & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & | & 0 \end{bmatrix}.$$

Next, we determine the solvability (feasibility or in feasibility) of the system using the rank and solvability Theorem. The rank(A) = rank[A|b] = number of unknowns = 6. Since, rank(A) = rank [A|b] = number of unknowns, the rank and solvability theorem implies that the system has a unique solution. Thus $Rx = 0$ becomes

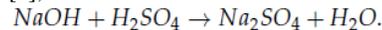
$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Hence, $u = v = w = x = y = z = 0$. Therefore, the system has a unique solution which is the zero solution. The main reason for given this example is because the conclusion given by Hamid [9] was 'vague.' This put the records straight about the in feasibility of the above reaction in his paper.

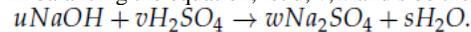
In the next two examples, we see the import of this present work in the sense that only (wx)maxima, gave rational forms of the Row Reduced Echelon Form of the resultant matrices. Matlab/Octave gave the rational numbers as floats.

3.2 Example

Sodium Hydroxide (NaOH) reacts with sulfuric acid (H_2SO_4) to yield sodium sulfate (Na_2SO_4) and water, the chemical reaction is as thus [9],



In balancing the equation, let u, v, w and s be the unknown variables such that



Comparing the number of Sodium(Na), Oxygen(O), Sulphur(S) and Hydrogen(H) atoms of the reactants with the number of atoms of the product, we obtain four (4) linear equations:

$$Na: \quad u = 2w$$

$$O: \quad u + 4v = 4w + s$$

$$H: \quad u + 2v = 2s$$

$$S: \quad v = w.$$

Rewriting these equations in standard form, we have a homogeneous linear system $Ax = 0$ of equations with four unknowns, u, v, w and s

$$\begin{bmatrix} 1 & 0 & -2 & 0 \\ 1 & 4 & -4 & -1 \\ 1 & 2 & 0 & -2 \\ 0 & 1 & -1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

$$\text{where } A = \begin{bmatrix} 1 & 0 & -2 & 0 \\ 1 & 4 & -4 & -1 \\ 1 & 2 & 0 & -2 \\ 0 & 1 & -1 & 0 \end{bmatrix}, \quad x = \begin{bmatrix} u \\ v \\ w \\ s \end{bmatrix} \text{ and } 0 \in \mathbb{R}^{4 \times 1}.$$

INPUT:

(%i5) A:matrix([1,0,-2,0], [1,4,-4,-1], [1,2,0,-2], [0,1,-1,0]);

INPUT:

(%i6) rref(A);

Yielding a row reduced echelon form of the form,

$$\sim \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

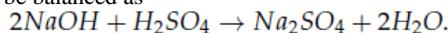
The rank(A) = 3, rank [A|b] = 3, and the number of unknowns = 4. By using the rank and solvability theorem, we see that rank(A) = rank[A|b] < number of unknowns. Thus, the system has infinitely many solutions. Hence, $\mathbf{R}\mathbf{x} = \mathbf{0}$ becomes

$$\begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & 0 & -\frac{1}{2} \\ 0 & 0 & 1 & -\frac{1}{2} \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

and $u - x = 0 \Rightarrow u = x, v - \frac{1}{2}s = 0 \Rightarrow v = \frac{1}{2}s, w - \frac{1}{2}s = 0 \Rightarrow w = \frac{1}{2}s$. Thus, the nullspace solution gives

$$\mathbf{x} = \begin{bmatrix} u \\ v \\ w \\ s \end{bmatrix} = \begin{bmatrix} s \\ \frac{1}{2}s \\ \frac{1}{2}s \\ s \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{2} \\ 1 \end{bmatrix} s.$$

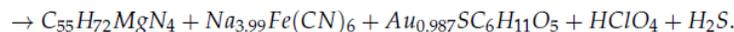
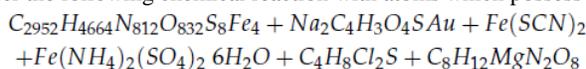
There are three pivot variables u, v and w and one free variable s. To avoid fractions, we set $s = 2$, so that $u = 2, v = 1, w = 1$. We remark that this is not the only solution since there is a free variable s, the nullspace solution is infinitely many. Hence, the chemical equation can be balanced as



Since there are infinitely many solutions to the resultant linear system, another choice of $s = 4$ would yield $u = 2, v = w = 2$, which still balances the chemical reaction.

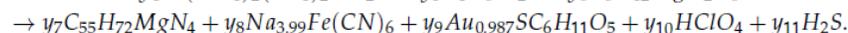
3.3 Example

Consider the following chemical reaction with atoms which possess fractional oxidation numbers [9]



In balancing the equation, let $y_1, y_2, y_3, y_4, y_5, y_6, y_7, y_8, y_9, y_{10}$ and y_{11} be the unknown variables such that

$$y_1\text{C}_{2952}\text{H}_{4664}\text{N}_{812}\text{O}_{832}\text{S}_8\text{Fe}_4 + y_2\text{Na}_2\text{C}_4\text{H}_3\text{O}_4\text{SAu} + y_3\text{Fe}(\text{SCN})_2 \\ + y_4\text{Fe}(\text{NH}_4)_2(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O} + y_5\text{C}_4\text{H}_8\text{Cl}_2\text{S} + y_6\text{C}_8\text{H}_{12}\text{MgN}_2\text{O}_8 \quad (1)$$



Next, we compare the number of Carbon(C), Hydrogen(H), Nitrogen(N), Oxygen(O), Sulphur(S), Iron(Fe), Sodium(Na), Gold(Au), Chlorine(Cl) and Magnesium (Mg) atoms respectively of the reactants with the number of atoms of the product. We obtained ten (10) linear system of equations in eleven (11) unknowns viz:

$$\text{C} : 2952y_1 + 4y_2 + 2y_3 + 4y_5 + 8y_6 = 55y_7 + 6y_8 + 6y_9$$

$$\text{H} : 4664y_1 + 3y_2 + 20y_4 + 8y_5 + 12y_6 = 72y_7 + 11y_9 + y_{10} + 2y_{11}$$

$$\text{N} : 812y_1 + 2y_3 + 2y_4 + 2y_6 = 4y_7 + 6y_8$$

$$\text{O} : 832y_1 + 4y_2 + 14y_4 + 8y_6 = 5y_9 + 4y_{10}$$

$$\text{S} : 8y_1 + y_2 + 2y_3 + 2y_4 + y_5 = y_9 + y_{11}$$

$$\text{Fe} : 4y_1 + y_3 + y_4 = y_8$$

$$\text{Na} : 2y_2 = 3.99y_8$$

$$\text{Au} : y_2 = 0.987y_9$$

$$\text{Cl} : 2y_5 = y_{10}$$

$$\text{Mg} : y_6 = y_7.$$

Rewriting these equations in standard form, we see a homogeneous linear system of equations in eleven unknowns;

$$\begin{aligned}
2952y_1 + 4y_2 + 2y_3 + 4y_5 + 8y_6 - 55y_7 - 6y_8 - 6y_9 &= 0 \\
4664y_1 + 3y_2 + 20y_4 + 8y_5 + 12y_6 - 72y_7 - 11y_9 - y_{10} - 2y_{11} &= 0 \\
812y_1 + 2y_3 + 2y_4 + 2y_6 - 4y_7 - 6y_8 &= 0 \\
832y_1 + 4y_2 + 14y_4 + 8y_6 - 5y_9 - 4y_{10} &= 0 \\
8y_1 + y_2 + 2y_3 + 2y_4 + y_5 - y_9 - y_{11} &= 0 \\
4y_1 + y_3 + y_4 - y_8 &= 0 \\
2y_2 - 3.99y_8 &= 0 \\
y_2 - 0.987y_9 &= 0 \\
2y_5 - y_{10} &= 0 \\
y_6 - y_7 &= 0.
\end{aligned}$$

The augmented matrix of the system of equations is

$$[A|b] = \left[\begin{array}{cccccccccccc|c}
2952 & 4 & 2 & 0 & 4 & 8 & -55 & -6 & -6 & 0 & 0 & 0 & 0 \\
4664 & 3 & 0 & 20 & 8 & 12 & -72 & 0 & -11 & -1 & -2 & 0 & 0 \\
812 & 0 & 2 & 2 & 0 & 2 & -4 & -6 & 0 & 0 & 0 & 0 & 0 \\
832 & 4 & 0 & 14 & 0 & 8 & 0 & 0 & -5 & -4 & 0 & 0 & 0 \\
8 & 1 & 2 & 2 & 1 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 \\
4 & 0 & 1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & -3.99 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -0.987 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0
\end{array} \right]$$

Using (wx)maxima in the input-output form,

INPUT:

```
(%i8) A: matrix( [2952,4,2,0,4,8,-55,-6,-6,0,0,0,0], [4664,3,0,20,8,12,-72,0,-11,-1,-2], [812,0,2,2,0,2,-4,-6,0,0,0,0,0],
[832,4,0,14,0,8,0,0,-5,-4,0,0,0], [8,1,2,2,1,0,0,0,-1,0,-1], [4,0,1,1,0,0,0,-1,0,0,0], [0,2,0,0,0,0,0,-3.99,0,0,0,0],
[0,1,0,0,0,0,0,-0.987,0,0], [0,0,0,0,2,0,0,-1,0], [0,0,0,0,1,-1,0,0,0,0] );
```

INPUT:

```
(%i9) rref(A);
```

OUTPUT:

rat: replaced -3.99 by -399/100 = -3.99rat: replaced -0.987 by -987/1000 = -0.987

We obtained in split seconds, the following Row Reduced Echelon Form of A:

$$\sim \left[\begin{array}{cccccccccccc|c}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{30448582}{16286436267} \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{3611102684}{5428812089} \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1299862196}{5428812089} \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{469616228}{5428812089} \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{5568665015}{16286436267} \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{1379870764}{16286436267} \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -\frac{1379870764}{16286436267} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -\frac{5430229600}{16286436267} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -\frac{10975996000}{16286436267} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -\frac{11137330030}{16286436267}
\end{array} \right]$$

Observe that because $\text{rank}(A) = \text{rank}([A|b]) = 10$ and less than the number of unknowns, the rank and solvability theorem guarantees the existence of infinitely many solutions. Also note that (wx)maxima magnanimously gave us fractional coefficients in the Row Reduced Echelon Form of A.

This implies that

