

Balancing Chemical Equations by Systems of Linear Equations

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Abstract

In this paper, a formal and systematic method for balancing chemical reaction equations was presented. The results satisfy the law of conservation of matter, and confirm that there is no contradiction to the existing way(s) of balancing chemical equations. A chemical reaction which possesses atoms with fractional oxidation numbers that have unique coefficients was studied. In this paper, the chemical equations were balanced by representing the chemical equation into systems of linear equations. Particularly, the Gauss elimination method was used to solve the mathematical problem with this method, it was possible to handle any chemical reaction with given reactants and products.

Keywords

Chemical Reaction, Linear Equations, Balancing Chemical Equations, Matrix, Gauss Elimination Method

1. Introduction

Balancing of the chemical equation is one of the initial subjects taught in most preliminary chemistry courses. Balancing chemical reactions is an amazing subject of matter for mathematics and chemistry students who want to see the power of linear algebra as a scientific discipline [1]. Since the balancing of chemical reactions in chemistry is a basic and fundamental issue, it deserves to be considered on a satisfactory level [2]. A chemical equation is only a symbolic representation of a chemical reaction. Actually, every chemical equation is the story of some chemical reaction. Chemical equations play a main role in theoretical as well as in industrial chemistry [3]. A chemical reaction can neither create nor destroy atoms. So, all of the atoms represented on the left side of the arrow must also be on the right side of the arrow. This is called balancing the chemical equa-

tion [4]. The application of the law of conservation of matter is critical in chemistry education and is demonstrated in practice through balanced chemical equations [5]. Every student who has general chemistry as a subject is bound to come across balancing chemical equations. 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 [6]. A chemical equation is said to be balanced, the number of atoms of each type on the left is the same as the number of atoms of corresponding type on the right [7].

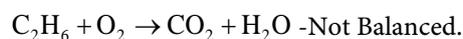
Balancing chemical equation by inspection is often believed to be a trial and error process and, therefore, it can be used only for simple chemical reactions. But still it has limitations [8]. Balancing by inspection does not produce a systematic evaluation of all of the sets of coefficients that would potentially balance an equation. Another common method of balancing chemical reaction equations is the algebraic approach. In this approach, coefficients are treated as unknown variables or undetermined coefficients whose values are found by solving a set of simultaneous equations [9]. According to [5], the author clearly indicated that the algebraic approach to balancing both simple and advance chemical reactions typically encountered in the secondary chemistry classroom is superior to that of the inspection method. Also, in [10], the author emphasized very clearly that balancing chemical reactions is not chemistry; it is just linear algebra. From a scientific viewpoint, a chemical reaction can be balanced if only it generates a vector space. That is a necessary and sufficient condition for balancing a chemical reaction.

A chemical reaction, when it is feasible, is a natural process, the consequent equation is always consistent. Therefore, we must have nontrivial solution. 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 a trivial solution, *i.e.*, all coefficients are equal to zero [6]. In Mathematics and Chemistry, there are several mathematical methods for balancing chemical reactions. All of them are based on generalized matrix inverses and they have formal scientific properties that need a higher level of mathematical knowledge for their application [1]-[16]. Here, we are presenting the Gauss elimination method, it was possible to handle any chemical reaction with given reactants and products. Solved problems are provided to show that this methodology lends well for both simple and complex reactions.

2. Main Results

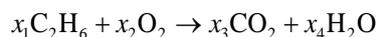
Problem 1

Balance the following chemical reaction



The equation to balance is identified. This chemical reaction consists of three elements: Carbon(C); Hydrogen (H); Oxygen (O). The equation to balance is

identified our task is to assign the unknowns coefficients (x_1, x_2, x_3, x_4) to each chemical species. A balance equation can be written for each of these elements:



Three simultaneous linear equations in four unknown corresponding to each of these elements. Then, the algebraic representation of the balanced

$$\text{Carbon (C): } 2x_1 = x_3 \Rightarrow 2x_1 - x_3 = 0$$

$$\text{Hydrogen (H): } 6x_1 = 2x_4 \Rightarrow 6x_1 - 2x_4 = 0$$

$$\text{Oxygen (O): } 2x_2 = 2x_3 + x_4 \Rightarrow 2x_2 - 2x_3 - x_4 = 0$$

First, note that there are four unknowns, but only three equations. The system is solved by Gauss elimination method as follows:

$$\begin{aligned} & \left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array} \right] \xrightarrow{R_2 \leftrightarrow R_2 - 3R_1} \left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 0 & 0 & 3 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array} \right] \\ & \xrightarrow{R_2 \leftrightarrow R_3} \left[\begin{array}{cccc|c} 2 & 0 & -1 & 0 & 0 \\ 0 & 2 & -2 & -1 & 0 \\ 0 & 0 & 3 & -2 & 0 \end{array} \right] \xrightarrow{\begin{array}{l} R_2 \leftrightarrow 3R_2 + 2R_3 \\ R_1 \leftrightarrow 3R_1 + R_3 \end{array}} \left[\begin{array}{cccc|c} 6 & 0 & 0 & -2 & 0 \\ 0 & 6 & 0 & -7 & 0 \\ 0 & 0 & 3 & -2 & 0 \end{array} \right] \\ & \xrightarrow{\begin{array}{l} R_1 \leftrightarrow \frac{1}{6}R_1 \\ R_2 \leftrightarrow \frac{1}{6}R_2 \\ R_3 \leftrightarrow \frac{1}{3}R_3 \end{array}} \left[\begin{array}{cccc|c} 1 & 0 & 0 & -1/3 & 0 \\ 0 & 1 & 0 & -7/6 & 0 \\ 0 & 0 & 1 & -2/3 & 0 \end{array} \right] \end{aligned}$$

The last matrix is of reduced row echelon form, so we obtain that the solution of the system of linear equations is:

$$x_1 - \frac{1}{3}x_4 = 0 \Rightarrow x_1 = \frac{1}{3}x_4$$

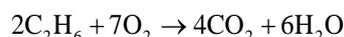
$$x_2 - \frac{7}{6}x_4 = 0 \Rightarrow x_2 = \frac{7}{6}x_4$$

$$x_3 - \frac{2}{3}x_4 = 0 \Rightarrow x_3 = \frac{2}{3}x_4$$

where x_4 a free variable, particular solution is can then obtain by assigning values to the x_4 , for instance $x_4 = 6$ we can represent the solution set as:

$$x_1 = 2, \quad x_2 = 7, \quad x_3 = 4$$

Thus, the balanced chemical reaction equation is:



Problem 2

Consider this chemical reaction which is infeasible



A balance equation can be written for each of these elements:



From above equation, we will obtain the following set of equations:

$$\text{K} : 4x_1 + 2x_2 = 2x_4$$

$$\text{Fe} : x_1 = x_6$$

$$\text{C} : 6x_1 = x_3$$

$$\text{N} : 6x_1 = 2x_5$$

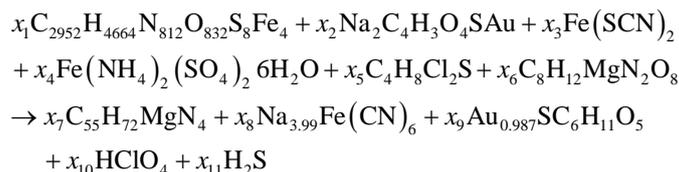
$$\text{S} : 2x_2 = x_4 + x_6$$

$$\text{O} : 3x_2 = 2x_3 + 4x_4 + 2x_5$$

From the systems of equations we obtain the contradictions $x_2 = 3x_1$ and $x_2 = \frac{44}{3}x_1$, that means that the system is inconsistent, *i.e.*, we have only a trivial solution $x_i = 0 (1 \leq i \leq 6)$. Hence, that means the chemical reaction is infeasible.

Problem 3

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



For balancing of this kind of reaction the computer is useless. From the mass balance of the above chemical reaction one obtains this system of linear equations

$$2952x_1 + 4x_2 + 2x_3 + 4x_5 + 8x_6 = 55x_7 + 6x_8 + 6x_9$$

$$4664x_1 + 3x_2 + 20x_4 + 8x_5 + 12x_6 = 72x_7 + 11x_9 + x_{10} + 2x_{11}$$

$$812x_1 + 2x_3 + 2x_4 + 2x_6 = 4x_7 + 6x_8$$

$$832x_1 + 4x_2 + 14x_4 + 8x_6 = 5x_9 + 4x_{10}$$

$$8x_1 + x_2 + 2x_3 + 2x_4 + x_5 = x_9 + x_{11}$$

$$4x_1 + x_3 + x_4 = x_8$$

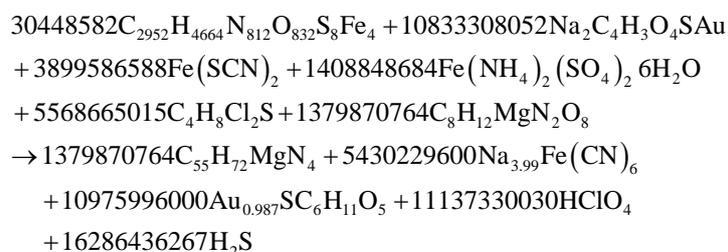
$$2x_2 = 3.99x_8$$

$$x_2 = 0.987x_9$$

$$2x_5 = x_{10}$$

$$x_6 = x_7$$

By using of the method of the elimination of the variables, from the chemical reaction and the system of linear equations immediately follows the required coefficients



Is it chemistry? No! It is linear algebra.

3. Results

Every chemical reaction can be represented by the systems of linear equations. A chemical reaction, when it is feasible, the consequent equation is always consistent. Therefore, we must have nontrivial solution. If the reaction is infeasible, then, there exists only a trivial solution, *i.e.*, all coefficients are equal to zero. A chemical reaction which possesses atoms with integers and fractional oxidation numbers was studied. And with this method, it was possible to handle any chemical reaction.

4. Conclusion

Balancing chemical reaction is not chemistry, but it is just linear algebra. This study investigates that every chemical reaction is represented by homogeneous systems of linear equations only. This allows average, and even low achieving students, a real chance at success. It can remove what is often a source of frustration and failure and that turns students away from chemistry. Also, it allows the high achieving to become very fast and very accurate even with relatively difficult equations. This work presented a formal, systematic approach for balancing chemical equations. The method is based on the Gaussian elimination method. The mathematical method presented in this paper was applicable to all cases in chemical reactions. The results indicated that there is no any contradiction between the various methods that were applied to balance the chemical reaction equation and the suggested approach. Balancing chemical reactions which possess atoms with fractional oxidation numbers is possible only by using mathematical methods.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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