



A NEW APPROACH TO BALANCING CHEMICAL EQUATIONS BY MATRIX ALGEBRA

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ABSTRACT

In this paper, we are using Mathematical model to balance Chemical equation. Particularly we are using Gauss elimination method and Gauss-Jordan method to balance the given chemical reaction equation. With this method, it is possible to balance any chemical reaction with given reactants and products.

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INTRODUCTION

A chemical equation shows the chemical formulas of substances that are reacting and the substances that are produced. The number of atoms of the reactants and products need to be balanced. In this lesson, we will discuss balancing chemical equations. We can see that it is unbalanced, with the right (red) side, weighing more than the left (blue) side. In order for the two sides to be balanced, we need to put a little more mass on the left side until they are the same mass. Just like we want the scale to be balanced on both sides, a chemical equation should also be balanced on both sides. A chemical equation shows us the substances involved in a chemical reaction - the substances that react (reactants) and the substances that are produced (products). In general, a chemical equation looks like this. According to the Gauss Elimination method, when a chemical reaction occurs, the mass of the products should be equal to the mass of the reactants. Therefore, the amount of the atoms in each element does not change in the chemical reaction. As a result, the chemical equation that shows the chemical reaction needs to be balanced. A balanced chemical equation occurs when the number of the atoms involved in the reactants side is equal to the number of atoms in the products side. This process is very useful in Industrial Chemistry. Every student which has general chemistry as a subject is bound to come across balancing chemical equations. Some authors [1-15] are balance chemical equations some different methods.

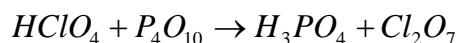
Chemical equations play great role in theoretical as well as industrial chemistry. Mass balance of chemical equations as a century old problem is one of the most highly studied topics in chemical education base on the rule called the law of conservation of matter, which states that atoms are not created or destroyed in a chemical reaction. It always has the biggest interest for science students on every level. The qualitative and quantitative understanding of the chemical process estimating reactants, predicting the nature and amount of products and determining reaction conditions is necessary to balance the chemical equation. Every student which has general chemistry as a subject is bound to come across balancing chemical equations.

Here we are presenting the Gauss Elimination method of balancing chemical equation using which we can easily determine whether the given chemical reaction exists or does not exists.

Mathematical Modeling of Chemical Reaction

Balancing the chemical reaction through Gauss Elimination method

The chemical equation is;



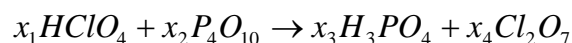
It is unbalance chemical equation, in this reaction there are four compounds

(H- Hydrogen; O-Oxygen; Cl-Chloride; P-Phosphorus).

To balance this equation, we insert unknowns, multiplying the reactants and the products to get an equation of the form

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Corresponding to eight compounds we have the eight simultaneous linear equations as below

$$H : x_1 = 3x_3$$

$$Cl : x_1 = 2x_4$$

$$O : 4x_1 + 10x_2 = 4x_3 + 7x_4$$

$$P : 4x_2 = x_3$$

It is important to note that we made use of the subscripts because they count the number of atoms of a particular element. Rewriting these equations in standard form, we see that we have a homogenous linear system in four unknowns, that is x_1, x_2, x_3, x_4

$$x_1 - 3x_3 = 0$$

$$x_1 - 2x_4 = 0$$

$$4x_1 + 10x_2 - 4x_3 - 7x_4 = 0$$

$$4x_2 - x_3 = 0$$

This is a homogeneous system of four linear equations in four unknowns. This system can be solved by Gauss elimination method.

Gauss elimination method:

Consider the matrix equation $AX=O$

$$\text{where } A = \begin{bmatrix} 1 & 0 & -3 & 0 \\ 1 & 0 & 0 & -2 \\ 4 & 10 & -4 & -7 \\ 0 & 4 & -1 & 0 \end{bmatrix}$$

$$X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \quad O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Now we obtain the echelon form of the matrix A as below:

Writing this equations or system in matrix form, we have the augmented matrix

$$A = \begin{bmatrix} 1 & 0 & -3 & 0 \\ 1 & 0 & 0 & -2 \\ 4 & 10 & -4 & -7 \\ 0 & 4 & -1 & 0 \end{bmatrix}$$

Solving augmented Matrix using Gauss Elimination method
By applying row reductions we get the echelon form

$$\begin{bmatrix} 1 & 0 & -3 & 0 \\ 0 & 10 & 8 & 7 \\ 0 & 0 & 3 & -2 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

From this we have

$$x_1 - 3x_3 = 0;$$

$$10x_2 + 8x_3 - 7x_4 = 0$$

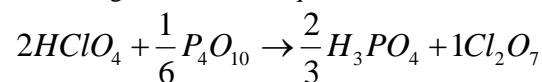
$$3x_3 - 2x_4 = 0$$

Suppose if

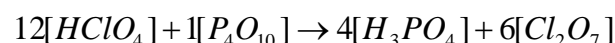
$$x_4 = 1, \text{ we get}$$

$$x_1 = 2, x_2 = \frac{1}{6}, x_3 = \frac{2}{3}, x_4 = 1$$

Now the given chemical equation becomes

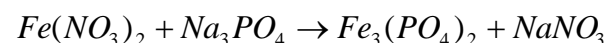


or



Balancing the chemical reaction through Gauss Jordan method

Consider the following unbalanced chemical reaction[15]

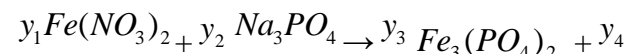


In this reaction, there are five compounds

1.Fe- Ferrous 2.N- Nitrogen 3. O-Oxygen 4.Na- Sodium
5.P- Phosphorus

The problem of balancing chemical equation is nothing but finding the coefficient for both reactants and products. we represent the above chemical reaction into the mathematical model form as below.

Suppose the required coefficient numbers are y_1, y_2, y_3, y_4 such that



Corresponding to five compounds we have the five simultaneous linear equations as below.

$$O : 6y_1 + 4y_2 = 8y_3 + 3y_4$$

$$N : y_1 = y_4$$

$$Fe : y_1 = 3y_3$$

$$Na : 3y_2 = y_4$$

$$P : y_2 = 2y_3$$

That is

$$y_1 - 3y_3 = 0$$

$$2y_1 - y_4 = 0$$

$$6y_1 + 4y_2 - 8y_3 - 3y_4 = 0$$

$$3y_2 - y_4 = 0$$

$$y_2 - 2y_3 = 0$$

More precisely

$$y_1 + 0y_2 - 3y_3 - 0y_4 = 0$$

$$2y_1 + 0y_2 - 0y_3 - y_4 = 0$$

$$6y_1 + 4y_2 - 8y_3 - 3y_4 = 0$$

$$0y_1 + 3y_2 - 0y_3 - y_4 = 0$$

$$0y_1 + y_2 - 2y_3 - 0y_4 = 0$$

This is a homogeneous system of five linear equations in four unknowns. This system can be solved by Gauss Jordan method.

Gauss Jordan method:

Consider the matrix equation $AX=O$

$$\text{where } A = \begin{bmatrix} 1 & 0 & -3 & 0 \\ 2 & 0 & 0 & -1 \\ 6 & 4 & -8 & -3 \\ 0 & 3 & 0 & -1 \\ 0 & 1 & -2 & 0 \end{bmatrix}$$

$$X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \quad O = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Now we obtain the echelon form of the matrix A as below:

$$A = \begin{bmatrix} 1 & 0 & -3 & 0 \\ 0 & 1 & -2 & 0 \\ 0 & 0 & 6 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

From this we have

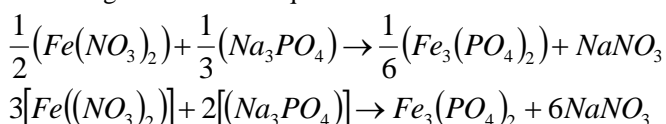
$$y_1 = 3y_3; \quad y_2 = 2y_3; \quad 6y_3 = y_4$$

Suppose if

$$y_4 = 1, \text{ we get}$$

$$y_1 = \frac{1}{2}, y_2 = \frac{1}{3}, y_3 = \frac{1}{6}, y_4 = 1$$

Now the given chemical equation becomes



RESULTS

1. Every chemical reaction can be represented by the matrix equation $AX = O$ where A is called a reaction matrix and X is a column matrix of coefficients X_i and O is a null column matrix.

2. If the matrix equation $AX = O$ has only trivial solution then corresponding chemical reaction is called infeasible reaction.
3. If the matrix equation $AX = O$ has non trivial solution then corresponding chemical reaction is called feasible reaction.

CONCLUSION

This method allows average, and even low level students, a real chance at success. It can remove what is often a source of frustration and failure that turns students away from chemistry. Also, it allows the high achieving to become very fast and very accurate even with relatively difficult equations. A balancing technique based on augmented-matrix protocols was described in this work. Because of its unusual nature, it was best explained through demonstration in the methodology. The practical superiority of the matrix procedure as the most general tool for balancing chemical equations is demonstrable. In other words, the mathematical method given here is applicable for all possible cases in balancing chemical equations.

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