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BALANCING CHEMICAL EQUATIONS BY USING MATRIX ALGEBRA

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ABSTRACT: In this paper, we describe a procedure employing Echelon form in Matrix Algebra to balance chemical equations. With this method, it is possible to handle any chemical reaction with given reactants and products.

KEYWORDS: Balancing Chemical equations, Chemical Reaction, Matrix, simultaneous Linear equations, Products.

1. INTRODUCTION

Unbalancing the chemical equations transform to balancing chemical equations, this process is very useful in Industrial Chemistry.

Every chemical equation is the story of some chemical reaction. The substances initially involved in a chemical reaction are called the reactants and newly formed substances are called products. Every student which has general chemistry as a subject is bound to come across balancing chemical equations. Every chemical equation should represent the Stoichiometry observed in the chemical reaction. 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. If some simple chemical reaction which cannot be balanced is given to balance it by using trial and error method then it becomes very difficult to conclude that such type of reactions do not happen physically. Some authors [1],[2],[5],[6],[10],[13],[14],[15] are balance chemical equations some different methods.

The balancing of chemical equations can be made much easier, especially for those who find it difficult, by moving the procedures toward the algorithmic and away from the heuristic. That is, a “step to step” procedure is simpler to master than is the haphazard hopping of inspection, even a highly refined inspection .[11] A popular, casual approach of coping with the challenges of balancing chemical-reaction equations is "by inspection".[3][4] The standard balancing-by-inspection approach is to make successive, hopefully intelligent guesses at the coefficients that will balance an equation, continuing until balance is achieved. This can be a straightforward, speedy approach for simple equations. But it rapidly becomes both lengthy and requires more skill for complex reactions that involve many reactants and products that require balancing.

Basically, the substances taking part in a chemical reaction are represented by their molecular formulae, and their symbolic representation is termed as chemical equation.[9] Chemical equation therefore is an expression showing symbolic representation of the reactants and the products usually positioned on the left side and on right side in a particular chemical reaction .[12] Unlike mathematical equations, left side and right side of chemical equations are usually separated using a single arrow pointing to the direction of the products for cases of one way reactions which are most times irreversible whereas a double arrow pointing either direction indicating a reversible reaction.[7] 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.

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

2. Mathematical Modeling of Chemical Reaction

The chemical equation is

$$K_4Fe(CN)_6 + KMnO_4 + H_2SO_4 \rightarrow KHSO_4 + Fe_2(SO_4)_3 + MnSO_4 + HNO_3 + CO_2 + H_2O$$

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

(C: Carbon; H- Hydrogen; N-Nitrogen; O-Oxygen; K: Potassium; Fe: Ferrum; Mn: Manganese; S: Sulfur).

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

$$y_1K_4Fe(CN)_6 + y_2KMnO_4 + y_3H_2SO_4 \rightarrow \begin{bmatrix} y_4KHSO_4 + y_5Fe_2(SO_4)_3 + y_6MnSO_4 \\ +y_7HNO_3 + y_8CO_2 + y_9H_2O \end{bmatrix}$$

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

K: $4y_1 + y_2 = y_4$

Fe: $y_1 = 2y_5$

C: $6y_1 = y_8$

N: $6y_1 = y_7$

Mn: $y_2 = y_6$

O: $4y_2 + 4y_3 = 4y_4 + 12y_5 + 4y_6 + 3y_7 + 2y_8$

H: $2y_3 = y_4 + y_7 + 2y_9$

S: $y_3 = y_4 + 3y_5 + y_6$

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 nine unknowns, that is $y_1, y_2, \ldots\ldots, y_9$

$$4y_1 + y_2 - y_4 = 0$$

$$y_1 - 2y_5 = 0$$

$$6y_1 - y_8 = 0$$

$$6y_1 - y_7 = 0$$

$$y_2 - y_6 = 0$$

$$4y_2 + 4y_3 - 4y_4 - 12y_5 - 4y_6 - 3y_7 - 2y_8 = 0$$

$$2y_3 - y_4 - y_7 - 2y_9 = 0$$

$$y_3 - y_4 - 3y_5 - y_6 = 0$$

We write these equations or system in matrix form, $AX = O$

$$\begin{bmatrix} 4 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 4 & 4 & -4 & -12 & -4 & -3 & -2 & 0 \\ 0 & 0 & 2 & -1 & 0 & 0 & -1 & 0 & -2 \\ 0 & 0 & 1 & -1 & -3 & -1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \\ y_7 \\ y_8 \\ y_9 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Now, we have the augmented matrix [AB]

$$\begin{bmatrix} 4 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 6 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 4 & 4 & -4 & -12 & -4 & -3 & -2 & 0 & 0 \\ 0 & 0 & 2 & -1 & 0 & 0 & -1 & 0 & -2 & 0 \\ 0 & 0 & 1 & -1 & -3 & -1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Solving augmented Matrix using Echelon form

By applying row reductions we get the echelon form

$$\begin{bmatrix} 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & -3 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -8 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 12 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -4 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 47 & -15 & 0 \end{bmatrix}$$

Converting into equations, we get

$$47y_8 - 15y_9 = 0$$

$$y_7 - y_8 = 0$$

$$-4y_6 + 3y_7 + 2y_8 + y_9 = 0$$

$$12y_5 - y_8 = 0$$

$$y_4 - 8y_5 - y_6 = 0$$

$$y_3 - y_4 - 3y_5 - y_6 = 0$$

$y_2 - y_4 + 8y_5 = 0$

$y_1 - 2y_5 = 0$

Take $y_1 = 10$, Substituting reversible equations,

We obtain $y_2 = 122, y_3 = 299, y_4 = 162, y_5 = 5, y_6 = 122, y_7 = 60, y_8 = 60, y_9 = 188$

In this case our balance equation is

$$10K_4Fe(CN)_6 + 122\,KMnO_4 + 299\,H_2SO_4 \rightarrow \begin{bmatrix} 162\ KHSO_4 + \ 5\,Fe_2(SO_4)_3 + 122\ MnSO_4 \\ +\ 60\ HNO_3 + \ 60\ CO_2 + 188\ H_2O \end{bmatrix}$$

3. RESULTS

- 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.
- If the matrix equation $AX = 0$ has only trivial solution then corresponding chemical reaction is called infeasible reaction.
- If the matrix equation $AX = 0$ has non-trivial solution then corresponding chemical reaction is called feasible reaction.

4. CONCLUSION

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 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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