Use of Gauss-Jordan Elimination Method to Balance Chemical Reaction

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Abstract

This paper gives a technique to balancing chemical reaction using the well-known method Gauss-Jordan Elimination method of linear algebra. Chemical reactions are combinations of Mathematical and Symbolic representation. Therefore, it is governed by specific rules and principles. The total number of atoms in a balanced reaction will be the same on both side of the reaction. The law of Conservation of mass states that the mass is the same before and after a chemical reaction. In a chemistry, balancing a chemical reaction is one of the most important issue. Many students and researcher used trial and error technique to balanced chemical reaction.

The Gauss –Jordan Elimination method of Linear algebra was used in solving the problem for balancing chemical reaction manually.

Keywords: balancing chemical reaction, Gauss-Jordan Elimination Method.

Introduction:

The law of conservations of mass tells us that the total amount of matter is neither created nor destroyed during any physical or chemical change. Therefore, the mass stays the same before and after a chemical reaction. Chemical equations demonstrate this principle because they are always balanced. The total mass of the reactants must same the total mass of the products.

Balancing an equation means adjust the coefficients until there are the same number of each type of atom on both sides. Balancing chemical reaction is one of the most important and preliminary in chemistry. , Balancing a chemical reaction is one of the basic requirements in chemistry. According to the Risteski , chemical reaction is "A symbolic representation and represents expressions of chemical elements and compounds or ions", where the reactants are given to the left side of the reaction and the product on the right side of the reaction.. Generally, balancing a chemical reaction is the mathematical problem. The students who does not know mathematical skill have difficulty in topics related to the balancing reaction. The aim of this paper is balancing chemical reaction using Gauss-Jordan elimination method of linear algebra.

Methodology:

1.Consider unbalanced chemical reaction.

2.For balancing the chemical reactions, assign the variables as the coefficient of each chemical compound to both side of the reactions.

3.For each chemical element in the reaction creates the linear equations.

4.The matrix A whose rows are the coefficient of variables of each linear equation. Let A be the m x n matrix, in which m is the number of rows i.e. number of elements and n be the number of columns i.e. number of chemical compounds.

Definition: Row Reduced Echelon form:

A m x n matrix is said to be row reduced echelon matrix if

1)The first non-zero element in each row of the matrix is unity.i.e. known as pivot or leading element.

2)The leading element of each row should be to the right of previous leading element.

3)A column has leading element, then its remaining element should be zero.

4)A row whose all elements are zero, it should be bottom of the matrix.

Definition: Augmented Matrix: let A be m x n matrix. Consider system of linear equation in matrix form written as AX=B. where X is n x 1 variable matrix and B is n x 1 constant matrix. The matrix [A, B] of order m x (n+1) is known as augmented matrix.

Definition: Rank of a matrix: Let A be m x n matrix. The rank of A is the number of non-zero rows in row reduced echelon matrix of A.

Definition: Elementary Transformation: Any matrix is reduced to another matrix by using the following transformation is known as elementary row transformation. There are three elementary row transformation as

i) Interchange i^{th} and j^{th} row of matrix by R_{ij}

ii) A non-zero scalar k multiply to i^{th} row by kR_i

iii) Scalar multiple of j^{th} row added in i^{th} row by $R_i + k\ R_j$

Gauss-Jordan Elimination Method:

Let A be m x n matrix and X be a n x 1 variable matrix. This method is used to solve the system of linear equations AX=B by applying following steps:

Step-1: Consider the system of linear equation in matrix form as AX=B.

Step-2: Construct the augmented matrix [A, B].

Step-3: Reduce the matrix [A, B] to row reduced echelon matrix [R, B']by applying elementary transformations.

Step-4: If rank(R)=rank ([R, B'] =n, then the system of linear equation AX=B has unique solution. If rank(R)=rank ([R, B'] < n then system of linear equations has infinitely many solutions. If rank(R)≠rank ([R, B']) then the system of linear equations has no solutions.

Problem-1. The methane CH_4 and oxygen O_2 reacts with each other produces carbon dioxide CO_2 and water H_2O.

$$CH_4 + O_2 \rightarrow CO_2 + H_2O \quad \text{(Unbalanced)}$$

Solution: To balance the given reaction, assign unknown variables x_1, x_2, x_3, x_4 to each chemical compounds of the given reaction as,

$$x_1\, CH_4 + x_2\, O_2 \rightarrow x_3\, CO_2 + x_4\, H_2O \qquad \text{……………………….. (1)}$$

Compare the number of atoms of carbon (C), hydrogen (H), oxygen (O) in reactants side with the number of atoms of product side. The linear equations from the above reaction (1) are as follows:

Carbon(C): $x_1 = x_3$ i.e. $x_1 - x_3 = 0$

Hydrogen (H): $4x_1 = 2\, x_4$ i.e. $4x_1 - 2\, x_4 = 0$

Oxygen (O): $2x_2 = 2x_3 + x_4$ i.e. $2x_2 - 2x_3 - x_4 = 0$

The given linear equations be written in matrix form as AX=B

$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 4 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \text{………(2)}$$

Consider augmented matrix

$$[A\,|B] = \left[\begin{matrix} 1 & 0 & -1 & 0 \\ 4 & 0 & 0 & -2 \\ 0 & 2 & -2 & -1 \end{matrix} \left|\begin{matrix} 0 \\ 0 \\ 0 \end{matrix}\right.\right]$$

By applying elementary transformation $R_2 - 4R_1$, R_{12}, $\frac{1}{2}R_2$, $\frac{1}{2}R_3$, $R_2 + R_3$, $R_2 + R_3$ on the augmented matrix [A|B], this matrix reduced to row reduced echelon form as

$$\left[\begin{matrix} 1 & 0 & 0 & -0.5 \\ 0 & 1 & 0 & -1 \\ 0 & 0 & 1 & -0.5 \end{matrix} \left|\begin{matrix} 0 \\ 0 \\ 0 \end{matrix}\right.\right] \text{… … … ..(3)}$$

Here rank (A) = 3= rank ([A, B]) < n=4, System (2) has infinitely many solutions. Let one variable x_4 is independent i.e. Free i.e.it takes any real number.

Let us consider $\boldsymbol{x_4 = 2}$,

Equations from the matrix (3) are as

From first row of matrix (3): $x_1 - 0.5x_4 = 0$ i.e. $x_1 - 0.5(2) = 0$ i.e $\boldsymbol{x_1 = 1}$

From second row of matrix (3): $x_2 - x_4 = 0$ i.e. $x_2 - 2 = 0$ i.e. $\boldsymbol{x_2 = 2}$

From third row of matrix (3): $x_3 - 0.5x_4 = 0$ i.e. $x_3 - 0.5(2) = 0$ i.e. $\boldsymbol{x_3 = 1}$

Hence unbalance reaction (1) reduced to balanced reaction which is

$$1\, CH_4 + 2O_2 \rightarrow 1\, CO_2 + 2\, H_2O$$

Problem-2:(Gas Evolving Reaction) A gas evolving reaction is a chemical process that produces a gas, such as oxygen or carbon dioxide. A nitric acid HNO3 reacts with sodium carbonate Na_2CO_3 to form sodium nitrate $NaNO_3$, carbon dioxide CO_2 and water H2O.

$$HNO_3 + Na_2CO_3 \rightarrow NaNO_3 + CO_2 + H_2O \text{ (Unbalanced)}$$

Solution: To balance this reaction, assign unknown variables x_1, x_2, x_3, x_4, x_5 to each chemical compounds as

$$x_1HNO_3 + x_2Na_2CO_3 \rightarrow x_3NaNO_3 + x_4CO_2 + x_5H_2O \qquad \text{…………… (4)}$$

Compare the number of atoms of hydrogen (H), nitrogen (N), oxygen (O), Sodium (Na), carbon (C) and in reactants with the number of atoms of product.

Hydrogen (H): $x_1 = 2x_5$ i.e. $x_1 - 2x_5 = 0$

Nitrogen (N): $x_1 = x_3$ i.e. $x_1 - x_3 = 0$

Oxygen (O): $3x_1 + 3x_2 = 3x_3 + 2x_4 + x_5$ i.e. $3x_1 + 3x_2 - 3x_3 - 2x_4 - x_5 = 0$

Sodium (Na): $2x_2 = x_3$ i.e. $2x_2 - x_3 = 0$

Carbon (C): $x_2 = x_4$ i.e. $x_2 - x_4 = 0$

The given linear equations be written in matrix form as AX=B

$$\begin{bmatrix} 1 & 0 & 0 & 0 & -2 \\ 1 & 0 & -1 & 0 & 0 \\ 3 & 3 & -3 & -2 & -1 \\ 0 & 2 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \ldots\ldots\ldots(5)$$

Consider augmented matrix

$$[A\,|B] = \begin{bmatrix} 1 & 0 & 0 & 0 & -2 & \Big| & 0 \\ 1 & 0 & -1 & 0 & 0 & \Big| & 0 \\ 3 & 3 & -3 & -2 & -1 & \Big| & 0 \\ 0 & 2 & -1 & 0 & 0 & \Big| & 0 \\ 0 & 1 & 0 & -1 & 0 & \Big| & 0 \end{bmatrix}$$

By applying elementary transformation $R_2 - R_1$, $R_3 - 3R_1, R_{25}$, $R_3 - R_2, R_4 - 2R_2, R_{34}$, $R_4 - 3R_3$, $R_5 - R_3, \frac{1}{5}R_4, \frac{1}{2}R_5$, $R_5 - R_4, R_2 - R_4, R_3 + 2R_4$, $-R_3, -R_4$ on the augmented matrix [A|B], this matrix reduced to row reduced echelon form as

$$\begin{bmatrix} 1 & 0 & 0 & 0 & -2 & \Big| & 0 \\ 0 & 1 & 0 & 0 & -1 & \Big| & 0 \\ 0 & 0 & 1 & 0 & -2 & \Big| & 0 \\ 0 & 0 & 0 & 1 & -1 & \Big| & 0 \\ 0 & 0 & 0 & 0 & 0 & \Big| & 0 \end{bmatrix} \ldots\ldots\ldots(6)$$

Here rank(A) = 4 = rank ([A, B]) < n = 5, Thus the system (5) has infinitely many solutions. Let one variable x_5 is independent variable, it takes any real number. Let $\boldsymbol{x_5 = 1}$, Equations from the matrix (6) are as:

From first row of matrix (6): $x_1 - 2x_5 = 0$ i.e. $\boldsymbol{x_1 = 2x_5 = 2}$

From second row of matrix (6): $x_2 - x_5 = 0$ i.e. $\boldsymbol{x_2 = x_5 = 1}$

From third row of matrix (6): $x_3 - 2x_5 = 0$ i.e. $\boldsymbol{x_3 = 2(x_5) = 2(1) = 2}$

From fourth row of matrix (6): $x_4 - x_5 = 0$ i.e. $\boldsymbol{x_4 = x_5 = 1}$

Hence unbalanced reaction (4) reduced to balanced reaction as

$$2HNO_3 + 1\ Na_2CO_3 \rightarrow 2NaNO_3 + 1\ CO_2 + 1\ H_2O$$

Conclusion:

In this paper, I have shown an easy and systematic approach for balancing a chemical reactions using Gauss-Jordan elimination method of Linear Algebra.

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