

# 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  $m \times n$  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  $m \times n$  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  $m \times n$  matrix. Consider system of linear equation in matrix form written as  $AX=B$ . where X is  $n \times 1$  variable matrix and B is  $n \times 1$  constant matrix. The matrix [A, B] of order  $m \times (n+1)$  is known as augmented matrix.

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

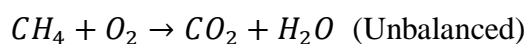
Step-1: Consider the system of linear equation in matrix form as  $AX=B$ .

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

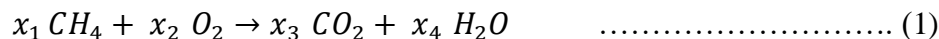
Step-3: Reduce the matrix [A, B] to row reduced echelon matrix [R, B'] by applying elementary transformations.

Step-4: If  $\text{rank}(R) = \text{rank}([R, B']) = n$ , then the system of linear equation  $AX=B$  has unique solution. If  $\text{rank}(R) = \text{rank}([R, B']) < n$  then system of linear equations has infinitely many solutions. If  $\text{rank}(R) \neq \text{rank}([R, B'])$  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  $H_2O$ .



**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,



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:

$$\text{Carbon(C): } x_1 = x_3 \quad \text{i.e. } x_1 - x_3 = 0$$

$$\text{Hydrogen (H): } 4x_1 = 2x_4 \quad \text{i.e. } 4x_1 - 2x_4 = 0$$

$$\text{Oxygen (O): } 2x_2 = 2x_3 + x_4 \quad \text{i.e. } 2x_2 - 2x_3 - x_4 = 0$$

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

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

Consider augmented matrix

$$[A|B] = \left[ \begin{array}{cccc|c} 1 & 0 & -1 & 0 & 0 \\ 4 & 0 & 0 & -2 & 0 \\ 0 & 2 & -2 & -1 & 0 \end{array} \right]$$

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

$$\left[ \begin{array}{cccc|c} 1 & 0 & 0 & -0.5 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & -0.5 & 0 \end{array} \right] \quad \dots\dots\dots (3)$$

Here  $\text{rank}(A) = 3 = \text{rank}([A, B]) < n=4$ , 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  $x_4 = 2$ ,

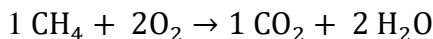
Equations from the matrix (3) are as

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

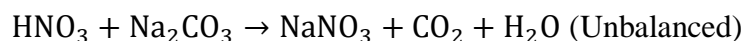
$$\text{From second row of matrix (3): } x_2 - x_4 = 0 \quad \text{i.e. } x_2 - 2 = 0 \quad \text{i.e. } x_2 = 2$$

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

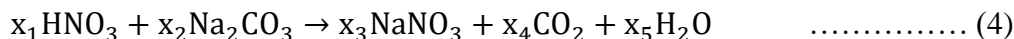
Hence unbalance reaction (1) reduced to balanced reaction which is



**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  $HNO_3$  reacts with sodium carbonate  $Na_2CO_3$  to form sodium nitrate  $NaNO_3$ , carbon dioxide  $CO_2$  and water  $H_2O$ .



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



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.

$$\text{Hydrogen (H):} \quad x_1 = 2x_5 \quad \text{i.e.} \quad x_1 - 2x_5 = 0$$

$$\text{Nitrogen (N):} \quad x_1 = x_3 \quad \text{i.e.} \quad x_1 - x_3 = 0$$

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

$$\text{Sodium (Na):} \quad 2x_2 = x_3 \quad \text{i.e.} \quad 2x_2 - x_3 = 0$$

$$\text{Carbon (C):} \quad x_2 = x_4 \quad \text{i.e.} \quad x_2 - x_4 = 0$$

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

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

Consider augmented matrix

$$[A|B] = \left[ \begin{array}{ccccc|c} 1 & 0 & 0 & 0 & -2 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 \\ 3 & 3 & -3 & -2 & -1 & 0 \\ 0 & 2 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \end{array} \right]$$

By applying elementary transformation  $R_2 - R_1, R_3 - 3R_1, R_5 - R_1, R_3 - R_2, R_4 - 2R_2, R_3 + R_4 - 3R_3, R_5 - R_3, \frac{1}{5}R_4, \frac{1}{2}R_5, R_5 - R_4, R_2 - R_4, R_3 + 2R_4, -R_3, -R_4$  on the augmented matrix  $[A|B]$ , this

matrix reduced to row reduced echelon form as

$$\left[ \begin{array}{ccccc|c} 1 & 0 & 0 & 0 & -2 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -2 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array} \right] \dots \dots \dots (6)$$

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

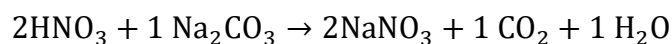
$$\text{From first row of matrix (6):} \quad x_1 - 2x_5 = 0 \quad \text{i.e.} \quad x_1 = 2x_5 = 2$$

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

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

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

Hence unbalanced reaction (4) reduced to balanced reaction as



### 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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