

An Overview on balancing chemical Equation Through Diophantine Equation

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Abstract: Diophantine equation is an algebraic polynomial with two or more unknowns and integer coefficients such that only the integral solutions are required. The Diophantine equation are used to solve for all unknowns in the problems. The Diophantine equation involves only sums, products and powers in which all the constants are integers and only solutions of interest are integers. There are many applications of Diophantine equations in various fields such as figuring out income over time, calculating mileage rates, predicting profit, calculating medicine doses based on patients' weights, real life geometric problems of physics, the field of cryptography, computational complexity theory, balancing the chemical reactions in chemistry, in this paper we discuss about the mathematical method of balancing chemical equations through Diophantine equations. Some examples are given in this paper in detail.

Key Word: Chemical Reaction, Diophantine equations, Balancing chemical Equations, molecular formula.

Introduction

Diophantine Equations:

There are two types of Diophantine equations, the linear and nonlinear Diophantine equations. The linear Diophantine equations is used all fields. In Chemistry it is used to solve chemical equation and molecular formula. If a, b, c are any given integers then the linear Diophantine with two variable is defined as $ax + by = c$.

Chemical Equation:

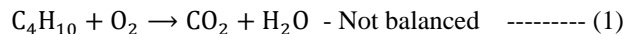
The chemical equation is a symbolic representation of chemical reaction consists of reactants on left side and products on right side with plus sign between both left side and right side and arrow towards the right side. In 1615 the first chemical equation was diagrammed by Jean Beguin.

Molecular formula:

An expression which states the number and type of atoms present in a molecule of a substance. Chemical reaction is a process that involves rearrangement of the molecular or ionic structure of a substance as distinct from a change in physical form or a nuclear reaction i.e., this is a process in which one or more substances the reactants are converted to one or more different substances the products. Substances are either chemical elements or compounds. There are many methods for balancing the chemical reactions.

1. Balance the chemical reaction:

Consider the unbalanced chemical reaction



This reaction consists of three elements, Carbon (C), Hydrogen (H) and Oxygen (O).

This chemical reaction is converted into mathematical form. Balancing the chemical reaction means finding the coefficients of both reactants and products. Given reaction consists of two reactants and two products then consider the four unknown coefficients (a, b, c, d) for both reactants and products. A balanced equation can be written as

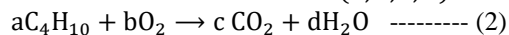


Table 1: Corresponding to four elements we have the coefficients are as follows:

Element	<i>a</i>	<i>b</i>	→	<i>c</i>	<i>d</i>
	Reactant			Products	
Carbon (C)	4	0	=	1	0
Hydrogen (H)	10	0	=	0	2
Oxygen(O)	0	2	=	2	1

Hence the algebraic representation of chemical reaction is

Carbon (C): $4a = c \Rightarrow 4a - c = 0$

Hydrogen(H): $10a = 2d \Rightarrow 10a - 2d = 0$

Oxygen(O): $2b = 2c + d \Rightarrow 2b - 2c - d = 0$

This is system of three homogeneous linear equations with four unknown constants.

1) Substitution Method:

The system of given linear equations can be written as,

$$4a - c = 0$$

$$5a - d = 0$$

Hence $c = 4a$ and $d = 5a$

Put these values in $2b - 2c - d = 0$ we get

$$2b - 2c - d = 0 \Rightarrow 2b - 8a - 5a = 0 \Rightarrow 2b = 13a \Rightarrow b = \frac{13}{2}a$$

Choose $a = 2$ we get $b = 13, c = 8$ and $d = 10$

2) The system is solved by Gauss elimination method as follows,

Consider the system of linear equations

$$4a - c = 0 \Rightarrow 4a + 0b - c + 0d = 0$$

$$2b - 2c - d = 0 \Rightarrow 0a + 2b - 2c - d = 0$$

$$5a - d = 0 \Rightarrow 5a + 0b + 0c - d = 0$$

Consider the matrix equation $AX = B$

Where $A = \begin{bmatrix} 4 & 0 & -1 & 0 \\ 0 & 2 & -2 & -1 \\ 5 & 0 & 0 & -1 \end{bmatrix}$, $X = \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$ and $B = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$

$$\left[\begin{array}{cccc|c} 4 & 0 & -1 & 0 & 0 \\ 0 & 2 & -2 & -1 & 0 \\ 5 & 0 & 0 & -1 & 0 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right]$$

Apply $\frac{1}{4}R_1, \frac{1}{2}R_2 \rightarrow$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1/4 & 0 & 0 \\ 0 & 1 & -1 & -1/2 & 0 \\ 5 & 0 & 0 & -1 & 0 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right]$$

Apply $R_3 - 5R_1 \rightarrow$

$$\left[\begin{array}{cccc|c} 1 & 0 & -1/4 & 0 & 0 \\ 0 & 1 & -1 & -1/2 & 0 \\ 0 & 0 & 5/4 & -1 & 0 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right] \text{----- (3)}$$

This shows that the given matrix is reduced to Echelon-Row form called Gauss Elimination converting into equations we get

$$\frac{5}{4}c - d = 0 \Rightarrow d = \frac{5}{4}c$$

$$a - \frac{1}{4}c = 0 \Rightarrow a = \frac{1}{4}c$$

$$b - c - \frac{1}{2}d = 0 \Rightarrow b = c + \frac{1}{2}d \Rightarrow b = c + \frac{5}{8}c \Rightarrow b = \frac{13}{8}c$$

Choose $c = 8 \Rightarrow a = 2, b = 13, d = 10$

1) The system is solved by Gauss-Jordan method as follows

Consider Echelon-Row form (from equation (3)) we have,

$$\left[\begin{array}{ccc|c} 1 & 0 & -1/4 & 0 \\ 0 & 1 & -1 & -1/2 \\ 0 & 0 & 5/4 & -1 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right] \text{----- (3)}$$

Apply $\frac{4}{5}R_3 \rightarrow$

$$\left[\begin{array}{ccc|c} 1 & 0 & -1/4 & 0 \\ 0 & 1 & -1 & -1/2 \\ 0 & 0 & 1 & -4/5 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right]$$

Apply $R_2 + R_3, R_1 + \frac{1}{4}R_3 \rightarrow$

$$\left[\begin{array}{ccc|c} 1 & 0 & 0 & -1/5 \\ 0 & 1 & 0 & -13/10 \\ 0 & 0 & 1 & -4/5 \end{array} \right] = \left[\begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right]$$

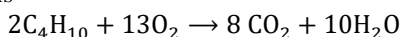
This shows that the given matrix is reduced to line-Echelon form called Gauss-Jordan Elimination Converting into equations we get

$$\begin{aligned} a - \frac{1}{5}d &= 0 \Rightarrow a = \frac{1}{5}d \\ b - \frac{13}{10}d &= 0 \Rightarrow b = \frac{13}{10}d \\ c - \frac{4}{5}d &= 0 \Rightarrow c = \frac{4}{5}d \end{aligned}$$

Choose $d = 10$ then $a = 2, b = 13$ and $c = 8$

This shows that in both the methods the values of unknown constant are same

For this variable the chemical reaction is



This shows that the chemical reaction is balanced

Result

Every chemical reaction can be represented by the system of linear equations can be represented by the matrix equation $AX = B$. Where A is called reaction matrix, X is the column matrix for variables (a, b, c, d) and B is the null matrix.

Conclusion

DwindiAgryantiJohar(1) says that the Gauss elimination and Gauss-Jordan methods are not suitable to apply balancing chemical reactions. From research it appears that the Substitution, Gauss elimination and Gauss-Jordan methods are suitable to apply balancing chemical reactions.

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