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BALANCING OF CHEMICAL EQUATIONS BY USING SIMULTANEOUS EQUATION AND MATRIX METHOD

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Abstract: In this paper we are trying to balance the chemical equations by representing the chemical equation in to the mathematical model. Particularly we are using the simultaneous linear equations method and Matrix to solve the mathematical problem. With this method, it is possible to handle any chemical reaction with given reactants and products.

Keywords: Chemical reaction, simultaneous linear equations, balancing chemical equations.

Introduction:

A chemical formula shows the number of atoms in a molecule. Chemical symbols and formula are combined together to form chemical equations, which explains a chemical equation. The problem of balancing chemical equation is nothing but finding the coefficient numbers for both reactants and products.

It has been noticed that some chemical equations cannot be balanced using trial and error method. Therefore simultaneous equation method and matrix is used. The procedures are as follows;

METHODOLOGY.

- i. **Simultaneous equation and**
- ii. **Matix method A^{-1} x B x det A**

<u>Question</u>

Balance the chemical equation of the decomposition reaction of 1,2,3-trinitroxypropane, or glyceryl trinitrate (Nitroglycerin)

$$C_3H_5(NO_3)_3 \rightarrow N_2 + O_2 + CO_2 + H_2O$$

PROCEDURE

- **Put coefficient a, b, c, d…, in front of each chemical formula, starting from reactants to products.**
- **For each element in the chemical equation, form a mathematical relation, i.e. L. H. S is equal to R. H. S,L. H. S. represents the total number of atoms of each type in the reaction, and R. H. S. represents the total number of atoms of each type in the product.**
- **Assume the first letter to be equal to unity, and then find other letter in terms of the first letter that was assumed to be unit.**
- **So we represent above chemical reaction into the mathematical form as shown below:**

SOLUTION

$$aC_3H_5(NO_3)_3 \qquad bN_2 + CO_2 + dCO_2 + eH_2O$$

For

$$\begin{aligned} &C: \quad 3a = d \ \ldots\ldots\ldots\ldots\ldots\ldots (1)\\ &H: \quad 5a = 2c \ \ldots\ldots\ldots\ldots\ldots\ldots (2)\\ &N: \quad 3a = 2b \ \ldots\ldots\ldots\ldots\ldots\ldots (3)\\ &O: \quad 9a = 2c + 2d + e \ \ldots\ldots\ldots (4) \end{aligned}$$

The equations above are then solved simultaneously (either by substitution or elimination)

Let a=1 (NOTE: when using this method the initial letter is always equal to 1)

Substitute the value of a=1 into equation (1), (2) and (3)
From equation 1

$$3a = d \qquad 3 \times 1 = d \qquad d = 3$$

From equation 2

$$5a = 2e \quad , \quad 5 \times 1 = 2e \quad ,$$

$$e = {}^{5}/_{2}$$

From equation 3

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3 x 1 =2b , 3 =2b

b =3/₂

From equation (4)

9 x 1=2c + 2 x3 + 5/2

9 =2c +6 +5/2 2c = 1/2

C =¼

Therefore we have that;
a= 1, b= 3/2, c= ¼, d= 3, e= 5/2.

$$C_3H_5(NO_3)_3 \rightarrow \frac{3}{2}N_2 + \frac{1}{4}O_2 + 3CO_2 + \frac{5}{2}H_2O$$

Multiply through by 4 to get the coefficient in whole number integer;

$$4C_3H_5(NO_3)_3 \rightarrow 6N_2 + O_2 + 12CO_2 + 10H_2O$$

BALANCING OF CHEMICAL EQUATIONS USING MATRIX.

In balancing of chemical equation using matrix, we talk about the stoichiometry matrix. In a chemical reaction, stoichiometry of the reaction is very important, that is the relationship between the numbers of moles of the reactants and the number of moles of the products.

STOICHIOMETRY MATRIX

i. **Balance the chemical reaction between Chromium and Oxygen using matrix.**

EQUATION OF REACTION

$$Cr + O_2 \rightarrow Cr_2O_3$$

SOLUTION

Following the above procedure, we rewrite the equation of reaction by introducing co-efficient. a, b and c.

$$aCr + bO_2 \rightarrow c\,Cr_2O_3$$

We have two different elements, Chromium and Oxygen so we need two different equations. We try to calculate the value of a, b and c the co-efficient of the reaction. The two equations look like this:

Cr: 1 a + 0 b = 2 c

O: 0 a + 2 b = 3c

We have two (2) matrices called Matrix A and B.

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad \text{and} \quad B = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

To obtain the value of a, b and c. the formula below will be use,

$$\begin{bmatrix} a \\ b \end{bmatrix} = A^{-1} \times [B] \times \det [A]$$

While the determinant of matrix A will be the value of c i.e det A = c

$$A^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad \text{and} \quad B = \begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

det A = 2 – 0 **therefore det A = 2 =c.**

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \; 3 \end{pmatrix} \begin{bmatrix} 2 \\ \end{bmatrix} \begin{bmatrix} 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 4 \\ \end{bmatrix}$$

Hence a =4 , b = 3 and c = 2.

Therefore, the equation of the reaction becomes

$$4\,Cr + 3O_2 \rightarrow 2Cr_2O_3$$

ii. **RESPIRATION REACTION: This the process of burning of carbohydrate through the help of Oxygen enzymes as catalyst to liberate carbon (iv) Oxide and Water.**

Equation of reaction:

$$C_6H_{12}O_6 + O_2 \underset{\text{Sunlight}}{\overset{\text{Enzymes}}{\rightleftharpoons}} H_2O + CO_2$$

SOLUTION

We rewrite the equation by introducing co-efficient a, b, c and d. therefore

$$aC_6H_{12}O_6 + bO_2 \underset{\text{Sunlight}}{\overset{\text{Enzymes}}{\rightleftharpoons}} c\,H_2O + dCO_2$$

Carbon : 6a + 0b = 1c + 0d : 6a + 0b + 1c = 0d
Hydrogen: 12a + 0b = 0c + 2d : 12a + 0b - 0c = 2d
Oxygen : 6a + 2b = 2c + 1d : 6a + 2b - 2c = 1d

The stoichiometry matrix of the equation of the reaction is

$$A = \begin{pmatrix} 6 & 0 & -1 \\ 12 & 0 & 0 \\ 6 & 2 & -2 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix}$$

Using the formula

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = (A)^{-1} \times (B) \times \det(A)$$

$$\det A = \left| 6(0-0)+0(-6+12)-1(24-0) \right| = -24 = d$$

$$A^{-1} = \begin{pmatrix} 0 & ½ & 0 \\ 1 & ¼ & ½ \\ 6 & ½ & 0 \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 & ½ & 0 \\ 1 & ¼ & ½ \\ 6 & ½ & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} (24) = \begin{pmatrix} -24/6 \\ -24 \\ -24 \end{pmatrix} = \begin{pmatrix} -4 \\ -24 \\ -24 \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} -4 \\ -24 \\ -24 \\ -24 \end{pmatrix}$$

multiply through by -1/4

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = -1/4 \begin{pmatrix} -4 \\ -24 \\ -24 \\ -24 \end{pmatrix} = \begin{pmatrix} 1 \\ 6 \\ 6 \\ 6 \end{pmatrix}$$

Hence, a = 1, b = 6 c = 6 and d= 6

There the balanced equation can be written as

$$C_6H_{12}O_6 + 6O_2 \underset{\text{Sunlight}}{\overset{\text{Enzymes}}{\rightleftharpoons}} 6\,H_2O + 6CO_2$$

Glucose oxygen water carbon (iv) oxide
This reversible reaction is called photosynthesis.

iii. The reaction between Magnesium Oxide and Iron to form Iron (ii) Oxide and Magnesium.

MgO + Fe → Fe2O3 + Mg

SOLUTION

We rewrite the equation by introducing co-efficient a, b, c and d. therefore

a MgO + bFe → cFe2O3 + dMg.

Mg: 1a + 0b = 0c + 1d : 1a + 0b + 0c = 1d

Fe: 0a + 1b = 2c + 0d : 0a + 1b - 2c = 0d

O: 1a + 0b = 3c + 0d : 1a + 0b - 3c = 0d

The stoichiometry matrix of the equation of the reaction is

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -2 \\ 1 & 0 & -3 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

det A = 1(-3-0)+0(0+2)- 0(0-1) = -3 = d

det A =d = -3

$$A^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2/3 & 1 & 2/3 \\ 1/3 & 0 & 1/3 \end{pmatrix}$$

Using the formula

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = (A)^{-1} \times [B] \times \det(A)$$

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 2/3 & 1 & 2/3 \\ 1/3 & 0 & 1/3 \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} (-3) = \begin{bmatrix} -3 \\ -2 \\ -1 \end{bmatrix}$$

Multiply through by -1

$$\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} 3 \\ 2 \\ 1 \\ 3 \end{bmatrix}$$

a = 3, b =2 , c = 1 , d = 3.
Hence, the balanced equation for the reaction is rewrite as

3 MgO + 2Fe → Fe2O3 + 3Mg.

IMPORTANCE OF CHEMICAL EQUATION

1. **It tells us the direction of the reaction and whether the reaction is reversible.**
2. **It tells us the individual elements and radicals involved.**
3. **It gives a mental picture of the movement of the element and radicals during the reactions.**

4. It tells us the state of matter in which the substance are present, as indicated by the state symbols-(S) for solid, (L) for liquid, (G) for gas, (aq) for aqueous solution which are placed after the formulae of the substances in the equation.

CONCLUSION

This paper has highlighted that every chemical equation 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. Some complex chemical reactions which cannot be balanced by inspection method or trial and error method are sometimes considered as reactions that cannot happen physically but here I showed that these complex chemical reactions can be balance using SIMULTANEOUS EQUATIONS AND MATRIX METHOD.

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