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Application of Mathematics in Balancing Chemical Equations

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Abstract: The mathematical model for balancing chemical equations is the topic of this research. The chemical equations in this work were balanced by converting them into systems of linear equations. The approach utilized to solve the system of linear equations is specifically the gauss elimination method. Any chemical reaction can be handled using this method as long as thereactantsand productsareknown.

I. INTRODUCTION

A chemical reaction occurs when one or more substances, known as reactants, are changed into one or more different substances, known as products. This is different from a change in physicalform or a nuclear reaction, which occurs when a substance rearranges its molecular or ionic structure. Chemical elements and compounds are classified as substances. In order to balance the chemical reaction, we employ the Gauss elimination method, one of several techniques for solving linear equations. The linear equation system is,

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2$$
$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n = b_3$$
$$\vdots$$
$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n$$

Or $$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Where a_{ij}
and $b_i$are known constants and
x_i are unknown constants.
The system of linear equations is equivalent to AX=B
Where A is Augmented Matrix, X is column vector of unknown constants and B is column vector of known constants.
The coefficient matrix was reduced to an upper triangular matrix and backward substitution was used in the Gauss elimination method. Procedure for applying the Gauss elimination method to solve linear equations. A diagonal matrix is created by reducing the coefficient matrix using the Gauss-Jordan method. Method steps for solving linear equations with the Gauss-Jordan method:
. Read the Augment Matrix A
. Reduce the augmented matrix [A/b] to the transform A into diagonal form.
. Divide right-hand side elements as well as diagonal elements by the diagonal elements in the row which will make each diagonal element equal to one.

II. GAUSS ELIMINATION METHOD

BALANCE THE CHEMICAL REACTION–BETWEEN COPPER AND NITRIC ACID

Consider the unbalanced chemical reaction

$$Cu + HNO_3 \rightarrow Cu(NO_3)_2 + NO + H_2O \qquad (1)$$

Thus (1) gives the not balanced chemical equation.

This reaction consists of four elements Copper(Cu), Hydrogen (H), Nitrogen(N) 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 three products then consider the five unknown coefficients (x_1,x_2,x_3,x_4,x_5) for

both reactants and products. A balanced equation can be written as

$$x_1Cu + x_2HNO_3 \rightarrow x_3Cu(NO_3)_2 + x_4NO + x_5H_2O \quad (2)$$

The algebraic representation of chemical reaction is Copper (Cu): $x_1 = x_3 \Rightarrow x_1 - x_3 = 0$

Hydrogen(H): $x_2 = 2x_5 \Rightarrow x_2 - 2x_5 = 0$

Nitrogen(N): $x_2 = 2x_3 + x_4 \Rightarrow x_2 - 2x_3 - x_4 = 0$

Oxygen(O): $3x_2 = 6x_3 + x_4 + x_5 \Rightarrow 3x_2 - 6x_3 - x_4 - x_5 = 0$

The system of linear equations can be written as,

$$\begin{aligned} x_1 + 0x_2 - x_3 + 0x_4 + 0x_5 &= 0 \\ 0x_1 + x_2 + 0x_3 + 0x_4 - 2x_5 &= 0 \\ 0x_1 + x_2 - 2x_3 - x_4 + 0x_5 &= 0 \\ 0x_1 + 3x_2 - 6x_3 - x_4 - x_5 &= 0 \end{aligned}$$

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

Consider the matrix equation AX=B

Where A=$\begin{bmatrix} 1 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 \\ 0 & 1 & -2 & -1 & 0 \\ 0 & 3 & -6 & -1 & -1 \end{bmatrix}$,X=$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$ and B=$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

The system is solved by Gauss elimination method as follows,

$$\Rightarrow \left[\begin{array}{ccccc|c} 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 1 & -2 & -1 & 0 & 0 \\ 0 & 3 & -6 & -1 & -1 & 0 \end{array}\right]$$

$$\Rightarrow \left[\begin{array}{ccccc|c} 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & -2 & -1 & 2 & 0 \\ 0 & 0 & -6 & -1 & 5 & 0 \end{array}\right] \begin{array}{l} R_3 \to R_3 - R_2 \\ R_4 \to R_4 - 3R_2 \end{array}$$

$$\Rightarrow \left[\begin{array}{ccccc|c} 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & -2 & -1 & 2 & 0 \\ 0 & 0 & 0 & 2 & -1 & 0 \end{array}\right] R_4 \to R_4 - 3R_3$$

$$\Rightarrow \left[\begin{array}{ccccc|c} 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -2 & 0 \\ 0 & 0 & -2 & -1 & 2 & 0 \\ 0 & 0 & 0 & 2 & -1 & 0 \end{array}\right]$$

The given matrix is reduced to Echelon-Row form Gauss Elimination equations we get

$$\begin{aligned} & x_1 - x_3 = 0 \Rightarrow x_1 = x_3 \\ & x_2 - 2x_5 = 0 \Rightarrow x_2 = 2x_5 \\ & -2x_3 - x_4 + 2x_5 = 0 \Rightarrow 2x_5 = 2x_3 + x_4 \\ & 2x_4 - x_5 = 0 \Rightarrow 2x_4 = x_5 \end{aligned}$$

Hence if $x_4 = \frac{1}{2}x_5$ then $x_2 = 2x_5, x_3 = \frac{3}{4}x_5, x_1 = \frac{3}{4}x_5$

Take $x_5 = 1$ then $x_4 = \frac{1}{2}, x_3 = \frac{3}{4}, x_2 = 2, x_1 = \frac{3}{4}$

Hence the chemical reaction equation (2) based on value of variables is

$$\left(\frac{3}{4}\right)Cu + 2HNO_3 \to \left(\frac{3}{4}\right)Cu(NO_3)_2 + \left(\frac{1}{2}\right)NO + H_2O$$

Take LCM on both sides in balancing chemical equations

$$3Cu + 8HNO_3 \to 3Cu(NO_3)_2 + 2NO + 4H_2O$$

III. GAUSS-JORDAN METHOD

BALANCE THE CHEMICAL REACTION –BETWEEN PLATINUM, NITRIC ACID AND HYDROCHLORIC ACID

Consider the unbalanced chemical reaction

$$Pt + HNO_3 + HCl \to NO + H_2(PtCl_6) + H_2O \qquad (3)$$

Thus (3) gives the not balanced chemical equation.

This reaction consists of five elements, Platinum (Pt), Hydrogen (H), Nitrogen (N), Oxygen (O),Chlorine(Cl).

This chemical reaction is converted into mathematical form. Balancing the chemical reactionmeans finding the coefficients of both reactants and products. Given reaction consists of three reactants and three products then consider the six unknown coefficients (x_1,x_2,x_3,x_4,x_5,x_6) for both reactants and products. A balanced equation can be written as

$$x_1Pt + x_2HNO_3 + x_3HCl \to x_4NO + x_5H_2(PtCl_6) + x_6H_2O \qquad (4)$$

The algebraic representation of chemical reaction is

Platinum (Pt): $x_1 = x_5 \Rightarrow x_1 - x_5 = 0$

Hydrogen(H): $x_2 + x_3 = 2x_5 + 2x_6 \Rightarrow x_2 + x_3 - 2x_5 - 2x_6 = 0$

Nitrogen(N): $x_2 = x_4 \Rightarrow x_2 - x_4 = 0$

Oxygen(O): $3x_2 = x_4 + x_6 \Rightarrow 3x_2 - x_4 - x_6 = 0$

Chlorine(Cl): $x_3 = 6x_5 \Rightarrow x_3 - 6x_5 = 0$

The system of linear equations can be written as,

$$\begin{aligned}
x_1 + 0x_2 + 0x_3 + 0x_4 - x_5 + 0x_6 &= 0 \\
0x_1 + x_2 + x_3 + 0x_4 - 2x_5 - 2x_6 &= 0 \\
0x_1 + x_2 + 0x_3 - x_4 + 0x_5 + 0x_6 &= 0 \\
0x_1 + 3x_2 + 0x_3 - x_4 + 0x_5 - x_6 &= 0 \\
0x_1 + 0x_2 + x_3 + 0x_4 - 6x_5 + 0x_6 &= 0
\end{aligned}$$

This is system of five homogeneous linear equations with six unknown constants.
Consider the matrix equation AX=B

Where A=$\begin{bmatrix} 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 1 & 0 & -2 & -2 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 3 & 0 & -1 & 0 & -1 \\ 0 & 0 & 1 & 0 & -6 & 0 \end{bmatrix}$, X=$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix}$ and B=$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

The system is solved by Gauss-Jordan method as follows

$$\Rightarrow \left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 & -2 & -2 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 3 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -6 & 0 & 0 \end{array}\right]$$

$$\Rightarrow \left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 & -2 & -2 & 0 \\ 0 & 0 & 1 & 1 & -2 & -2 & 0 \\ 0 & 0 & -3 & -1 & 6 & 5 & 0 \\ 0 & 0 & 1 & 0 & -6 & 0 & 0 \end{array}\right] \begin{array}{l} R_3 \to R_3 - R_2 \\ R_4 \to R_4 - 3R_2 \\ R_3 \to -R_3 \end{array}$$

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$$\Rightarrow\left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & -2 & -2 & 0 \\ 0 & 0 & 0 & 2 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 & -4 & 2 & 0 \end{array}\right] \begin{array}{l} R_2 \to R_2 - R_3 \\ R_4 \to R_4 + 3R_3 \\ R_5 \to R_5 - R_3 \end{array}$$

$$\Rightarrow\left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & -2 & -2 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -1 & -4 & 2 & 0 \end{array}\right] R_4 \to \frac{R_4}{2}$$

$$\Rightarrow\left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & -2 & -3/2 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & -4 & 3/2 & 0 \end{array}\right] \begin{array}{l} R_2 \to R_2 + R_4 \\ R_3 \to R_3 - R_4 \\ R_5 \to R_5 + R_4 \end{array}$$

$$\Rightarrow\left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & -2 & -3/2 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 1 & -3/8 & 0 \end{array}\right] R_5 \to \frac{-R_5}{4}$$

$$\Rightarrow\left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & 0 & -3/8 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & 0 & -9/4 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 1 & -3/8 & 0 \end{array}\right] \begin{array}{l} R_1 \to R_1 + R_5 \\ R_3 \to R_3 + 2R_5 \end{array}$$

$$\Rightarrow \left[\begin{array}{cccccc|c} 1 & 0 & 0 & 0 & 0 & -3/8 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1/2 & 0 \\ 0 & 0 & 1 & 0 & 0 & -9/4 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 1 & -3/8 & 0 \end{array}\right]$$

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

$$x_1 - \frac{3}{8}x_6 = 0 \Rightarrow x_1 = \frac{3}{8}x_6$$

$$x_2 - \frac{1}{2}x_6 = 0 \Rightarrow x_2 = \frac{1}{2}x_6$$

$$x_3 - \frac{9}{4}x_6 = 0 \Rightarrow x_3 = \frac{9}{4}x_6$$

$$x_4 - \frac{1}{2}x_6 = 0 \Rightarrow x_4 = \frac{1}{2}x_6$$

$$x_5 - \frac{3}{8}x_6 = 0 \Rightarrow x_5 = \frac{3}{8}x_6$$

Take $x_6 = 1$ then $x_1 = \frac{3}{8}, x_2 = \frac{1}{2}, x_3 = \frac{9}{4}, x_4 = \frac{1}{2}, x_5 = \frac{3}{8}$

This shows that in both the methods the values of unknown constant are same Hence the chemical reaction equation (4) based on value of variables are

$$\left(\frac{3}{8}\right)Pt + \left(\frac{1}{2}\right)HNO_3 + \left(\frac{9}{4}\right)HCl \rightarrow \left(\frac{1}{2}\right)NO + \left(\frac{3}{8}\right)H_2(PtCl_6) + H_2O$$

Take LCM on both sides in balancing chemical equation

$$3Pt + 4HNO_3 + 18HCl \rightarrow 4NO + 3H_2(PtCl_6) + 8H_2O$$

IV. CONCLUSION

Chemical reaction balancing is essentially linear algebra; it is not chemistry. This study examines into the concept that homogeneous systems of linear equations are the only representations ofevery chemical reaction. This gives mediocre and even low achievers a genuine opportunity at success. It can take away something which usually prompts learners to get frustrated and unsuccessful and to lose interest in chemistry.

Additionally, it makes great achievement possible even for sparingly difficult assignments, allowing very fast and precise results. A structured and methodical method for balancing chemical equations was introduced in this work. The Gaussian elimination approach forms the basis of the procedure .Any scenario involving chemical reactions could be solved using the mathematical approach described in this work. The findingsshowed that the suggested strategy and the different approaches used to balance the chemicalreaction equation do not contradict one other. Chemical processes involving atoms with fractional oxidation number scan only be balanced mathematically.

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