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Mathematical Model for balancing chemical Reaction

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Abstract
In this paper we discuss about the mathematical model for balancing chemical equations. In this paper the chemical equations were balanced by representing the chemical equation into systems of linear equations. Particularly the gauss elimination method is used to solve the system of linear equations. This method is possible to handle any chemical reaction with given reactants and products.

Keywords: Chemical Reaction, Linear equations, Balancing chemical Equations, Matrix, Gauss Elimination method

Introduction

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 solving the linear equations, here we use Gauss elimination method for balancing the chemical reaction. Consider the system of linear equations

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n = b_3$$

$$\vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n$$

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.

In the Gauss elimination method the coefficient matrix was reduced to an upper triangular matrix and the backward substitution was applied. Steps of solution of linear equations using Gauss elimination Method:

- Read the Augment Matrix A
- Reduce the matrix in upper triangular form.
- Use backward substitution to get the solution

In the Gauss-Jordan method the coefficient matrix is reduced into a diagonal matrix. Steps of solution of linear equations using 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.

Mathematical Modeling of chemical reaction:

A chemical equation is said to be balanced the number of atoms of corresponding type on the right. Here we discuss how a chemical reaction is balanced by representing as a system of linear equations.

Consider the unbalanced chemical reaction

$\mathrm{Pb} + \mathrm{PbO_2} + \mathrm{H_2}SO_4 \longrightarrow \mathrm{PbSO_4} + \mathrm{H_2O}$ - Not balanced --------- (1)

This reaction consists of four elements, Lead (Pb), Oxygen (O), Sulphur (S) and Hydrogen (H).

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 three reactants and two 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

$x_1\mathrm{Pb} + x_2\mathrm{PbO_2} + x_3\mathrm{H_2SO_4} \longrightarrow x_4\mathrm{PbSO_4} + x_5\mathrm{H_2O}$ --------- (2)

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

Element	x_1	x_2	x_3	$\longrightarrow$	x_4	x_5
	Reactants				Products	
Lead(Pb)	1	1	0	=	1	0
Oxygen(O)	0	2	4	=	4	1
Sulphur(S)	0	0	1	=	1	0
Hydrogen(H)	0	0	2	=	0	2

Hence the algebraic representation of chemical reaction is

Lead(Pb): $x_1 + x_2 = x_4 \Longrightarrow x_1 + x_2 - x_4 = 0$

Oxygen(O): $2x_2 + 4x_3 = 4x_4 + x_5 \Longrightarrow 2x_2 + 4x_3 - 4x_4 - x_5 = 0$

Sulphur(S): $x_3 = x_4 \Longrightarrow x_3 - x_4 = 0$

Hydrogen(H): $2x_3 = 2x_5 \Longrightarrow 2x_3 - 2x_5 = 0$

Hence the system of linear equations can be written as,

$$x_1 + x_2 + 0x_3 - x_4 + 0x_5 = 0$$

$$0x_1 + 2x_2 + 4x_3 - 4x_4 - x_5 = 0$$

$$0x_1 + 0x_2 + x_3 - x_4 + 0x_5 = 0$$

$$0x_1 + 0x_2 + 2x_3 + 0x_4 - 2x_5 = 0$$

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

Consider the matrix equation $AX = B$

Where $A = \begin{bmatrix} 1 & 1 & 0 & -1 & 0 \\ 0 & 2 & 4 & -4 & -1 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 2 & 0 & -2 \end{bmatrix}$, $X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix}$ and $B = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

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

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

Apply $R_4 - 2R_3 \longrightarrow$

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

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

$x_1 + x_2 - x_3 = 0 \Longrightarrow x_1 = -x_2 + x_3$

$2x_2 + 4x_3 - 4x_4 - x_5 = 0 \Longrightarrow 2x_2 = -4x_3 + 4x_4 + x_5 = 0$

$x_3 - x_4 = 0 \Longrightarrow x_3 = x_4$

$2x_4 - 2x_5 = 0 \Longrightarrow x_4 = x_5$

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

Take $x_5 = 2$ then $x_4 = 2$, $x_3 = 2$, $x_2 = 1$ and $x_1 = 1$

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

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

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

Apply $\frac{1}{2}R_2$ and $\frac{1}{2}R_4 \longrightarrow$

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

Apply $R_3 + R_4 \longrightarrow$

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

Apply $R_2 - 2R_3 + 2R_4 \longrightarrow$

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

Apply $R_2 - R_2 + R_4 \longrightarrow$

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

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

$x_1 - \frac{1}{2}x_5 = 0 \Longrightarrow x_1 = \frac{1}{2}x_5$

$x_2 - \frac{1}{2}x_5 = 0 \Longrightarrow x_2 = \frac{1}{2}x_5$

$x_3 - x_5 = 0 \Longrightarrow x_3 = x_5$

$x_4 - x_5 = 0 \Longrightarrow x_4 = x_5$

Take $x_5 = 2$ then $x_4 = 2$, $x_3 = 2$, $x_2 = 1$ and $x_1 = 1$

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

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

$\mathrm{Pb} + \mathrm{PbO_2} + 2\mathrm{H_2SO_4} \longrightarrow 2\mathrm{PbSO_4} + 2\mathrm{H_2O}$

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 x_i for $i = 1,2,3,4,5$ and B is the null matrix.

Conclusion: From research it appears that the Gauss elimination and Gauss-Jordan methods are suitable to apply balancing chemical reactions. Balancing chemical reaction is not a chemistry but it is mathematics.

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