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Application of System Linear Diophantine Equations in Balancing Chemical Equations

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Abstract: In this manuscript, the step by step procedure for how the system of linear Diophantine equations are applied to balance chemical equations acquired by the reactions of various chemical compounds and their products is scrutinized.
Keywords: Chemical equation, Linear Diophantine equation, Echelon form.

I. INTRODUCTION

The very basic concept of chemistry is balancing the chemical equation. Balancing means that the number of reactions is equal to the number of products. There are so many real-life applications of the Diophantine equations. In [1-3], the author delivers different branches of chemistry. In [4-10], the authors derived the balanced form of chemical equation using Gauss elimination methods. In this manuscript, the method of application simultaneous linear Diophantine equations in balancing chemical equations is studied.

II. TECHNIQUE FOR BALANCING CHEMICAL EQUATIONS

The detailed explanation of the application of system linear Diophantine equations in balancing chemical equations is illustrated through the following algorithm.

1) *Step 1:* Introduce the variables by multiplying the reactants and products in the unbalanced chemical equation.
2) *Step 2:* Develop a system of linear homogeneous equations by comparing the number of atoms of the actions with the number of reactions.
3) *Step 3:* Find the values of the variables by solving the equations developed in step 2 by suitable method.
4) *Step 4:* Substitution of the values of the newly introduced variables in the unbalanced equation in step2 results the equation into balanced.

A. *Some Examples are Deliberated Below*

1) *Example 1*

Consider the reaction of 2,4 −Dichlorophenoxy acetic acid ($C_8H_6Cl_2O_3$) with Hydrogen peroxide (H_2O_2) and oxygen (O_2) which yields hydrochloric acid(HCl), carbon dioxide (CO_2) and water (H_2O). The equivalent form unbalanced chemical equation is

$$\boldsymbol{C_8H_6Cl_2O_3 + H_2O_2 + O_2 \xrightarrow{Fe(III)} HCl + CO_2 + H_2O}\ .$$

The step by step procedure of converting this unbalanced equation into balanced equation is illustrated below.

a) *Step 1:* Introduce u, v, w, x, y and z are the unknowns to be multiplied in the reactants and products of the unbalanced equation as shown below.

$$u.C_8H_6Cl_2O_3 + v.H_2O_2 + w.O_2 \xrightarrow{Fe(III)} x.HCl + y.CO_2 + z.H_2O \qquad (1)$$

b) *Step 2:* Frame the system of linear homogenous equations with six unknowns by comparing the action and reaction of the equation (1) as follows.

Cl: $2u - x = 0$
O: $3u + 2v + 2w - 2y - z = 0$
H: $6u + 2v - x - 2z = 0$
C: $8u - y = 0$

The augmented matrix of the above system of equations is

$$\begin{array}{c} Cl \\ O \\ H \\ C \end{array}\begin{pmatrix} 2 & 0 & 0 & -1 & 0 & 0 & 0 \\ 3 & 2 & 2 & 0 & -2 & -1 & 0 \\ 6 & 2 & 0 & -1 & 0 & -2 & 0 \\ 8 & 0 & 0 & 0 & -1 & 0 & 0 \end{pmatrix}$$

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c) Step 3: Solving the equations by Gauss Elimination method. The Echelon form of the matrix presented in step 2 is given by

$$\begin{pmatrix} 8 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 2 & 2 & 0 & -13/8 & -1 & 0 \\ 0 & 0 & -2 & -1 & 19/8 & -1 & 0 \\ 0 & 0 & 0 & -1 & 1/4 & 0 & 0 \end{pmatrix}$$

d) Step 4: The reduced form of system of equations are evaluated by

$$-x + \frac{1}{4}y = 0$$
$$-2w - x + \frac{19}{8}y - z = 0$$
$$2v + 2w - \frac{13}{8}y - z = 0$$
$$8u - y = 0$$

The selections of $u = h_1$ and $z = h_2$ delivers the integer values of x, y, v and w as given below

$$x = 2h_1$$
$$y = 8h_1$$
$$v = h_2 - 2h_1$$
$$w = \frac{17h_1 - h_2}{2}$$

where $h_1 \in N$ and h_2 is an odd positive integer. Note that all the positive values of u, v, w, x, y, z are balancing the chemical equation mentioned in (1).
Limited balanced chemical equations for particular adoptions of h_1 and h_2 are registered in the table 2.1.

Table 2.1

h_1	h_2	u	v	w	x	y	z	Balanced chemical equations
1	3	1	1	7	2	8	3	$C_8H_6Cl_2O_3 + H_2O_2 + 7O_2 \to 2HCl + 8CO_2 + 3H_2O$
1	5	1	3	6	2	8	5	$C_8H_6Cl_2O_3 + 3H_2O_2 + 6O_2 \to 2HCl + 8CO_2 + 5H_2O$
2	6	2	2	14	4	16	6	$2C_8H_6Cl_2O_3 + 2H_2O_2 + 14O_2 \to 4HCl + 16CO_2 + 6H_2O$
3	7	3	1	22	6	24	7	$3C_8H_6Cl_2O_3 + H_2O_2 + 22O_2 \to 6HCl + 24CO_2 + 7H_2O$
3	9	3	3	21	6	24	9	$3C_8H_6Cl_2O_3 + 3H_2O_2 + 21O_2 \to 6HCl + 24CO_2 + 9H_2O$

2) Example 2

Consider the reaction of Silver (Ag) with Hydroxide (OH) and Formic acid $(HCOO)$ which produces silver (Ag), Carbonate (CO_3) and water (H_2O). Then the resultant unbalanced chemical equation is

$$\boldsymbol{Ag + OH + HCOO \to Ag + CO_3 + H_2O}$$

To balance the above unbalanced chemical equation, let us introduce the unknowns a, b, c, d, e and f in the chemical equation as exemplified below.

$$a.Ag + b.OH + c.HCO_2 \to d.Ag + e.CO_3 + f.H_2O \qquad (2)$$

Comparison of products and reactions provides the following system of linear equations.

$$Ag: a - b = 0$$
$$O: b + 2c - 3e - f = 0$$
$$H: b + c - 2f = 0$$
$$C: c - e = 0.$$

Solving the system of equations by Gauss Elimination method as in Example 1 by putting appropriate values for few variables, the choices of all other unknowns are received by

$a = h_2, b = 3h_1, c = h_1, d = h_2, e = h_1, f = 2h_1$, where $h_1, h_2 \in N$.

The positive solutions to the system equations and the collection of balanced equations for few chances of h_1 and h_2 are given in table 2.2.

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Table 2.2

h_1	h_2	a	b	c	d	e	f	Balanced chemical equations
1	2	2	3	1	2	1	2	$2Ag + 3OH + HCOO \rightarrow 2Ag + CO_3 + 2H_2O$
2	4	4	6	2	4	2	4	$4Ag + 6OH + 2HCOO \rightarrow 4Ag + 2CO_3 + 4H_2O$
3	2	2	9	3	2	3	6	$2Ag + 9OH + 3HCOO \rightarrow 2Ag + 3CO_3 + 6H_2O$
4	7	7	12	4	7	4	8	$7Ag + 12OH + 4HCOO \rightarrow 7Ag + 4CO_3 + 8H_2O$
6	1	1	18	6	1	6	12	$Ag + 18OH + 6HCOO \rightarrow Ag + 6CO_3 + 12H_2O$

3) Example 3:

Suppose Hydrogen bromide (HBr) reacts with Sulfuric acid (H_2SO_4) which produce Bromine(Br_2), Sulfur dioxide(SO_2) and water(HO_2). Then, the unbalanced chemical equation is monitored by

$$\boldsymbol{HBr + H_2SO_4 \longrightarrow H_2O + Br_2 + SO_2}. \qquad (3)$$

Let us introduce the unknowns a, b, c, d, e in the unbalanced chemical equation as follows.

$$a.HBr + b.H_2SO_4 \longrightarrow c.H_2O + d.Br_2 + e.SO_2$$

As in example 1 and 2, solve the following system of equations by Gauss Elimination method.

$H: a + 2b - 2c = 0$

$Br: a - 2d = 0$

$S: b - e = 0$

$O: 4b - c - 2e = 0.$

It is exposed by $a = 2h, b = h, c - 2h, d = h, e = h$ for all $h \in N$.

Table 2.3 displays the group of balanced equations for some values of h.

Table 2.3

h	a	b	c	d	e	Balanced chemical equations
1	2	1	2	1	1	$2HBr + H_2SO_4 \longrightarrow 2H_2O + Br_2 + SO_2$
2	4	2	4	2	2	$4HBr + 2H_2SO_4 \longrightarrow 4H_2O + 2Br_2 + 2SO_2$
3	6	3	6	3	3	$6HBr + 3H_2SO_4 \longrightarrow 6H_2O + 3Br_2 + 3SO_2$
4	8	4	8	4	4	$8HBr + 4H_2SO_4 \longrightarrow 8H_2O + 4Br_2 + 4SO_2$
5	10	5	10	5	5	$10HBr + 5H_2SO_4 \longrightarrow 10H_2O + 5Br_2 + 5SO_2$

4) Example 4

The reaction of Hydrogen iodide (HI) with Sulfuric acid (H_2SO_4) gives Iodine (I_2), Hydrogen Sulfide(H_2S) and water(H_2O). Here, the unstable chemical equation is of the form

$$\boldsymbol{HI + H_2SO_4 \longrightarrow H_2O + I_2 + H_2S}. \qquad (4)$$

Elect the newly introduced variables as l, m, n, o, p and resolve the following system of equations developed by the procedure as in example (1) by Gauss Elimination method. $H: \mathrm{l} + 2m - 2n - 2p = 0$

$I: l - 2o = 0$

$S: m - p = 0$

$O: 4m - n = 0$

Hence, $l = 8h, m = h, n = 4h, o = 4h$ and $p = h$, where $h \in N$.

Table 2.4 shows the values of the variables and cluster of balanced form of chemical equations for little bit choices of h.

Table 2.4

h	l	m	n	o	p	Balanced chemical equations
1	8	1	4	4	1	$8HI + H_2SO_4 \longrightarrow 4H_2O + 4I_2 + H_2S$
2	16	2	8	8	2	$16HI + 2H_2SO_4 \longrightarrow 8H_2O + 8I_2 + 2H_2S$
3	24	3	12	12	3	$24HI + 3H_2SO_4 \longrightarrow 12H_2O + 12I_2 + 3H_2S$
4	32	4	16	16	4	$32HI + 4H_2SO_4 \longrightarrow 16O + 16I_2 + 4H_2S$
5	40	5	20	20	5	$40HI + 5H_2SO_4 \longrightarrow 20H_2O + 20I_2 + 5H_2S$

5) Example 5

The reaction of Boron trifluoride (BF_3) with Sodium hydride (NaH) gives Boron hydride (B_2H_6) and Sodium fluoride (NaF).Then, $\boldsymbol{BF_3 + NaH \longrightarrow B_2H_6 + NaF}$ is an unstable chemical equation.

Following the same method as explained in example 1, frame the system of equations by introducing the variables p, q, r, s as shown below.

$B: p - 2r = 0$

$F: 3p - s = 0$

$Na: q - s = 0$

$H: q - 6r = 0$

The solutions to this system of equations are $p = 2h, q = 6h, r = h$ and $s = 6h$ where $h \in N$.

Possible positive solutions to the simultaneous equations and the equivalent balanced chemical equations are offered in table 2.5.

Table 2.5

h	p	q	r	s	Balanced chemical equations
1	2	6	1	6	$2BF_3 + 6NaH \longrightarrow B_2H_6 + 6NaF$
2	4	12	2	12	$4BF_3 + 12NaH \longrightarrow 2B_2H_6 + 12NaF$
3	6	18	3	18	$6BF_3 + 18NaH \longrightarrow 3B_2H_6 + 18NaF$
4	8	24	4	24	$8BF_3 + 24NaH \longrightarrow 4B_2H_6 + 24NaF$
5	10	30	5	30	$10BF_3 + 30NaH \longrightarrow 5B_2H_6 + 30NaF$

III. CONCLUSION

In this document, the analysis of how the system of linear Diophantine equations are used in balancing chemical equations assimilated by the reactions of various chemical combinations and their products is presented. In this way, one can search real life applications of higher degree Diophantine equations in various fields.

REFERENCES

[1] Steiner, Erich, "The chemistry maths book." Oxford University Press, 2008.
[2] Somorjai, Gabor A., and Yimin Li, "Introduction to surface chemistry and catalysis." John Wiley & Sons, 2010.
[3] Manahan, Stanley E., "Fundamentals of environmental chemistry." CRC press, 2011.
[4] Vishwambharrao, Kakde Rameshkumar, I. N. Raju, and H. S. Shivarudrappa. "Balancing chemical equations by using mathematical model." International Journal of Mathematical Research and Science, Vol 1, Issue 4, 2013, 129-132.
[5] Risteski, Ice B. , "A New Generalized Algebra for the Balancing of Chemical Reactions." Materials and Technology 48,Vol 2, 2014, 215-219.
[6] Gabriel, Cephas Iko-ojo, and Gerald Ikechukwu Onwuka, "Balancing of chemical equations using matrix algebra." Journal of Natural Sciences Research, Vol 5, No. 5, 2015, 29-36.
[7] Akinola, R. O., Kutchin, S. Y., Nyam, I. A., & Adeyanju, O. , "Using Row Reduced Echelon Form in Balancing Chemical Equations." Advances in Linear Algebra & Matrix Theory, Vol 6, 2016, 146-157.
[8] Padmaja, V., Y. Harikrishna, and G. V. Ramana Reddy , "An innovative approach of matrix algebra to balancing chemical-reaction equations." World of Journal of Pharmacy and Pharmaceutical Sciences, Vol 6, Issue 3, 2017, 260-266.
[9] Krishna, Y. Hari, N. Vijaya, and P. Bindu, "Balancing chemical equations using Gauss-Jordan Elimination aided by MATLAB." Journal of Xi'an University of Architecture & Technology, Vol 12, 2020, 347-352.
[10] Udawat, Bharat, "Gauss Jordan method for balancing chemical equation for different materials." Materials Today: Proceedings, Vol 51, 2022, 451-454.