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CHEMICAL REACTION DIOPHANTINE EQUATIONS

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ABSTRACT

The use of the linear diophantine equations to balance the valency number of the chemical equations is demonstrated in this study. Additionally, a few chemical equations and their balanced versions are shown.

Keywords: linear diophantine equations, chemical equations, Applications,

INTRODUCTION

When atoms gain or lose electrons to yield ions, or fuse with alternative atoms to make molecules, their symbols are changed or combined to get chemical formulas that fittingly represent some species. Extending this symbolism to represent each the identities and also the relative quantities of substances undergoing a chemical (or physical) amendment involves writing and reconciliation of a chemical equation. In view of a chemist a simplest and most generally used method for balancing chemical equations is by inspection or balancing them using molecular weight. When it comes to a mathematician, it is done effectively by treating it as equations and solve using various methods. Here the chemical equations are balanced using diophantine equations. Solving Diophantine equation is closely tied to standard arithmetic and number theory. A Diophantine equation within the kind $ax+by=c$ is a linear diophantine equations in 2 variables. If 2 comparatively prime integers a and b written during this kind with c = 1, the equation can associate infinite range of solutions. additionally there'll forever be associated infinite range of solutions if $\gcd(a,b)=1$, and there are not any solutions to the equation if $\gcd(a,b)\nmid c$.

In this paper various chemical reactions are considered and treated as linear diophantine equation and are balanced consequently.

Method of analysis:

Consider the chemical reaction of the form,

$$pu_{p'}v_{q'}w_{r'}+qu_{p''}v_{q''}w_{r''}+ru_{p'''}v_{q'''}w_{r'''}+\ldots=Pu_{P'}v_{Q'}w_{R'}+Qu_{P''}v_{Q''}w_{R''}+Ru_{P'''}v_{Q'''}w_{R'''}+\ldots \qquad (1)$$

(1) leads to,

$$\begin{aligned} pp'+qp''+rp'''+\ldots &= PP'+QP''+RP'''+\ldots \\ pq'+qq''+rq'''+\ldots &= PQ'+QQ''+RQ'''+\ldots \qquad (2) \\ pr'+qr''+rr'''+\ldots &= PR'+QR''+RR'''+\ldots \end{aligned}$$

where u, v and w, were the elements within the reaction, are positive integers or zero, and $p',q,',r',...P',Q',R',....$ indicates the unknown coefficients of the reactants and product. Equation (2) is an elementary Diophantine equation which gives all integer solutions [u, v, w, … U, V, W, …].

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$$pu_{p'}v_{q'}w_{r'} + qu_{p''}v_{q''}w_{r''} + ru_{p'''}v_{q'''}w_{r'''} + \ldots = Pu_{P'}v_{Q'}w_{R'} + Qu_{P''}v_{Q''}w_{R''} + Ru_{P'''}v_{Q'''}w_{R'''} + \ldots \quad (1)$$

(1) leads to,

$$\begin{aligned} pp'+qp''+rp''' + \ldots &= PP'+QP''+RP'''+\ldots \\ pq'+qq''+rq''' + \ldots &= PQ'+QQ''+RQ'''+\ldots \\ pr'+qr''+rr''' + \ldots &= PR'+QR''+RR'''+\ldots \end{aligned} \quad (2)$$

where u, v and w, were the elements in the reaction, $p', q', r', \ldots P', Q', R', \ldots$ are non-negative integers and p, q, r, … , P, Q, R, … are the determinable coefficients of the reactants and products.

Equation (2) is an elementary Diophantine equation which gives all integer solutions [u, v, w, … U, V, W, …].

Several chemical equations representing the formation of various chemical products and chemical biproducts are considered and the considered equations are balanced treating them as linear diophantine equations.

1. The following is the process of preparing Ethyl Alcohol from Molasses, which has been a procedure in the Trichy Distilleries and Chemicals Ltd., Trichy.

$$C_6H_{12}O_6 \xrightarrow{\text{zymase}} C_2H_5OH + CO_2$$

Rewriting the above equation gives,

$$pC_6H_{12}O_6 \xrightarrow{\text{zymase}} P\,C_2H_5OH + QCO_2 \quad (3)$$

Here p, P, and Q are the unknowns to be identified to balance the equation.
From (3), the following is obtained.

$$\left.\begin{aligned} &\text{For 'C'}, p = 2P + Q \\ &\text{For 'H'}, 12p = 6P \\ &\text{For 'O'}, 6p = P + 2Q \end{aligned}\right\} \quad (4)$$

(4) gives, 4p-2Q = 0.
This is a linear diophantine equation in two unknowns which in solving gives, [p, Q] = [1, 2].
Hence,

$$C_6H_{12}O_6 \xrightarrow{\text{zymase}} 2C_2H_5OH + 2CO_2$$

2. Wurtz Reaction:

$$CH_3Br + Na \rightarrow C_2H_6 + NaBr$$

$$pCH_3Br + qNa \rightarrow PC_2H_6 + QNaBr \quad (5)$$

Here p, q, P, and Q are the constants to be identified to balance the equation.
From (5) , the following is obtained.

$$\text{For 'C'}, p = 2P$$

$$\text{For 'H'}, 3u = 6P$$

$$\text{For 'Br'}, p = P$$

$$\text{For 'Na'}\ q = Q$$

which reduces to $p = q$.

This is a linear diophantine equation in two unknowns which in solving gives, [p, q] = [2, 2].

Hence,

$$2CH_3Br + 2Na \rightarrow C_2H_6 + 2NaBr$$

3. Kolbe's Reaction:
   Sodium acetate added to water and when electrolyzed gives ethane and bi-products.

$$CH_3COONa + H_2O \xrightarrow{Electrolysis} C_2H_6 + CO_2 + H_2 + NaOH$$

This equation is rewritten as,

$$pCH_3COONa + qH_2O \xrightarrow{Electrolysis} PC_2H_6 + QCO_2 + RH_2 + SNaOH \quad (6)$$

Here p, q, P, Q, R and S are the constants to be identified to balance the equation.
From (6), the following are obtained.

$$\left.\begin{aligned} &\text{For 'C'}, p = 2P + Q \\ &\text{For 'H'}, 3p + 2q = 6P + 2R + S \\ &\text{For 'O'}, 2p + q = 2Q + S \\ &\text{For 'Na'}, p = S \end{aligned}\right\} \quad (7)$$

(7) reduces to, $5p - 5q + 4R = 0$.

This is a linear diophantine equation in three unknowns which in solving gives, [p, q, R] = [2, 6, 5].
Thus [p, q, P, Q, R, S] = [2, 6, 1, 2, 5, 2].

Hence, $2CH_3COONa + 2H_2O \xrightarrow{Electrolysis} C_2H_6 + 2CO_2 + H_2 + 2NaOH$

4. Preparation of water from Methane:

$$CH_4 + O_2 \rightarrow CO + H_2 0$$

Now this equation is balanced treating this as a linear diophantine equation in three variables.
The considered equation is rewritten as,

$$pCH_4 + qO_2 \rightarrow PCO + QH_2 0 \quad (8)$$

where p, q, P, Q are the constants to be identified to balance the equation.
From (8), the following are obtained.

$$\left.\begin{aligned} &\text{For 'C'}, p = P \\ &\text{For 'H'}, 4p = Q \\ &\text{For 'O'}, 2q = P + Q \end{aligned}\right\} \quad (9)$$

(9) reduces to $3p - 2q = 0$.

This is a linear diophantine equation in two unknowns which in solving gives,
[p, q] = [2, 3].

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Thus [p, q, P, Q] = [2, 3, 2, 4].

Hence $2CH_4 + 3O_2 \rightarrow 2CO + 4H_2O$

5. Preparation of Manganese:

$$Mno_2 + Al \rightarrow Mn + Al_2O_3$$

Rewriting the above equation leads to,

$$pMno_2 + qAl \rightarrow PMn + QAl_2O_3 \qquad (10)$$

This on proceeding as in the previous cases reduces to,
2p -3q = 0.
From the above equation the basic solution is obtained as, [p, q] = [3, 2].
Thus [p, q, P, Q] = [3, 2, 3, 2].

Hence, $3Mno_2 + 2Al \rightarrow 3Mn + 2Al_2O_3$

S.No	Unbalanced equation	Balanced equation
1	$Zn + HCl \rightarrow ZnCl_2 + H_2$	$Zn + 2HCl \rightarrow ZnCl_2 + H_2$
2	$CaO + C \rightarrow CaC_2 + CO$	$CaO + 3C \rightarrow CaC_2 + CO$
3	$N_2 + H_2 \rightleftharpoons NH_3$	$N_2 + 3H_2 \rightleftharpoons 2NH_3$
4	$H_2 + I_2 \rightleftharpoons HI$	$H_2 + I_2 \rightleftharpoons 2HI$
5	$Al + Cl_2 \rightarrow AlCl_3$	$2Al + 3Cl_2 \rightarrow 2AlCl_3$
6	$Si + F_2 \rightarrow SiF_4$	$Si + 2F_2 \rightarrow SiF_4$
7	$CaCO_3 + HCl \rightarrow CaCl_2 + H_2O + CO_2$	$CaCO_3 + 2HCl \rightarrow CaCl_2 + H_2O + CO_2$
8	$BaCl_2 + Na_2SO_4 \rightarrow BaSO4 + NaCl$	$BaCl_2 + Na_2SO_4 \rightarrow BaSO_4 + 2NaCl$
9	$CuO + NH_3 \rightarrow Cu + N_2 + H_2O$	$3CuO + 2NH_3 \rightarrow 3Cu + N_2 + 3H_2O$
10	$HCl + O_2 \rightarrow H_2O + Cl_2$	$4HCl + O_2 \rightarrow 2H_2O + 2Cl_2$

CONCLUSION

There are several applications for diophantine equations. In this paper the linear diophantine equations are used to balance the valency number of chemical equations. One may also try to attempt some other procedures to do the same.

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