THE SEQUENTIAL PATTERN IN SOME COMBUSTION REACTIONS

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Due to different and specific relationships between chemical elements and their atoms, balancing of chemical equations can reach a high degree of complexity. Sometimes it can be insoluble. Intuitive methods, *i.e.* trial-and-error and oxidation-reduction, were developed to solve this problem. However, the balancing of chemical equations can be seen and worked in a mathematical perspective, given it deals with the reorganization of elements (atoms) into blocks of different constitutions (molecules). Therefore, this work presents a new methodology to balance chemical equations that represent combustion reactions. This new balancing strategy is based on numerical sequences and provides quick balancing for the chemical equations in question.

INTRODUCTION

When the combustion reaction of organic substances - that is, where the carbon element is the main constituent of the reactive molecules – are studied, a sequential pattern of the stoichiometric coefficients of the reagents and products present in the chemical equations is observed. This pattern can be seen as a numerical sequence that depends on the number of carbon atoms that constitute the molecules. In this perspective, a new methodology is proposed to find the unknown coefficients based on the application of the mathematical sequence theory to balancing some chemical equations that represent reactions of complete combustion suffered by some organic compounds. Using numerical sequences allows the chemist to determining the stoichiometric coefficients in a fast and easy way and to understand the repetition patterns that occur in different classes of chemical reactions.

IMPORTANT DEFINITIONS

DEFINITION 1: Complete Combustion (*burnout*)

$$\text{Organic Substance} + xO_2 \longrightarrow yCO_2 + zH_2O$$

Ex: $$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

DEFINITION 2: Infinit Sequence (*row*)
Function whose domain are integers

Ex:						
Domain:	1	2	3	...	n	(set of integers)
Image:	3	6	9	...	3n	(depends on n)
Sequence:	a_1	a_2	a_3	...	a_n	(terms of a row)

DEFINITION 3: Limited Sequence

- Top limited: If M which $a_n \leq M$ ∀ n
- Under limited: If P which $a_n \geq P$ ∀ n

⇒ Limited Sequence: $P \leq a_n \leq M$

DEFINITION 4: Convergence of a Sequence

- Convergent: If $\epsilon > 0$ exists N ∀ n: $n > N \Longrightarrow |a_n - L| < \epsilon \Longrightarrow \lim_{n\to\infty} a_n = L$
- Divergent: If $\epsilon > 0$ exists N ∀ n: $n > N \Longrightarrow |a_n - L| > \epsilon \Longrightarrow \lim_{n\to\infty} a_n = \nexists$

APPLICATION

Hydrocarbons

Alkane Combustion	Alkene Combustion
$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$	$C_2H_4 + 3O_2 \longrightarrow 2CO_2 + 2H_2O$
$C_2H_6 + {}^7/_2\, O_2 \longrightarrow 2CO_2 + 3H_2O$	$C_3H_6 + {}^9/_2\, O_2 \longrightarrow 3CO_2 + 3H_2O$
$C_3H_8 + 5O_2 \longrightarrow 3CO_2 + 4H_2O$	$C_4H_8 + 6O_2 \longrightarrow 4CO_2 + 4H_2O$
$C_4H_{10} + {}^{13}/_2\, O_2 \longrightarrow 4CO_2 + 5H_2O$	$C_5H_{10} + {}^{15}/_2\, O_2 \longrightarrow 5CO_2 + 5H_2O$
$C_5H_{12} + 8O_2 \longrightarrow 5CO_2 + 6H_2O$	$C_6H_{12} + 9O_2 \longrightarrow 6CO_2 + 6H_2O$
...	...
$a_nC_nH_{2n+2} + b_nO_2 \longrightarrow c_nCO_2 + d_nH_2O$	$a_nC_nH_{2n} + b_nO_2 \longrightarrow c_nCO_2 + d_nH_2O$

Oxygenated Functions

Alcohols Combustion	Carboxylic Acids Combustion
$CH_3OH + {}^3/_2\, O_2 \longrightarrow CO_2 + 2H_2O$	$CH_2O_2 + {}^1/_2\, O_2 \longrightarrow 1CO_2 + 1H_2O$
$C_2H_5OH + 3O_2 \longrightarrow 2CO_2 + 3H_2O$	$C_2H_4O_2 + 2O_2 \longrightarrow 2CO_2 + 2H_2O$
$C_3H_7OH + {}^9/_2\, O_2 \longrightarrow 3CO_2 + 4H_2O$	$C_3H_6O_2 + {}^7/_2\, O_2 \longrightarrow 3CO_2 + 3H_2O$
$C_4H_9OH + 6O_2 \longrightarrow 4CO_2 + 5H_2O$	$C_4H_8O_2 + 5O_2 \longrightarrow 4CO_2 + 4H_2O$
$C_5H_{11}OH + {}^{15}/_2\, O_2 \longrightarrow 5CO_2 + 6H_2O$	$C_5H_{10}O_2 + {}^{13}/_2\, O_2 \longrightarrow 5CO_2 + 5H_2O$
...	...
$a_nC_nH_{2n+1}OH + b_nO_2 \longrightarrow c_nCO_2 + d_nH_2O$	$a_nC_nH_{2n}O_2 + b_nO_2 \longrightarrow c_nCO_2 + d_nH_2O$

Sequencies Properties

Organic Functions	GENERAL TERMS OF ESTEQUIOMETRIC COEFFICIENTS				Properties
	Organic Substance	O_2	CO_2	H_2O	
Hydrocarbons Alkane	$a_n = 1$	$b_n = \frac{3n+1}{2}$	$c_n = n$	$d_n = n + 1$	- a_n is convergent and top limited.
Hydrocarbons Alkene	$a_n = 1$	$b_n = \frac{3n}{2}$	$c_n = n$	$d_n = n$	
Alcohols	$a_n = 1$	$b_n = \frac{3n}{2}$	$c_n = n$	$d_n = n + 1$	- b_n, c_n e d_n are divergents.
Carboxylic Acids	$a_n = 1$	$b_n = \frac{3n}{2}$	$c_n = n$	$d_n = n$	

CONCLUSION

The presented methodology is a new way of finding the stoichiometric coefficients of simple chemical reactions. Although this work has been limited to combustion reactions, methodology can be applied to other types of chemical reactions that shows a pattern in the stoichiometric coefficients.

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