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Using Mean Oxidation Number of Organic Carbons to Quantify Buswell's Equation

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Abstract

Buswell's equation can represent anaerobic digestion. The overall stoichiometric chemical equation is important for the counting of biomethane and theoretical biochemical methane potential. Although the concept of oxidation number of organic carbons has been applied in organic chemistry and biochemistry, the relationship between mean oxidation number of organic carbons and quantity of biomethane has not been studied. This article uses the H-atom method as a balancing tool to build a Buswell's model which can help understand the redox nature of organic compounds and establish the mathematical relationships among the stoichiometric coefficients of Buswell's equation, elemental composition of organic compound, and mean oxidation number of organic carbons. By using mean oxidation number of organic carbons as a metric, the mathematical equations for the counting of biomethane and theoretical biochemical methane potential are attained. The parameters of Buswell's equation can also be quantified by any given structural formula of an organic compound.

Keywords: anaerobic digestion, Buswell's equation, H-atom method, mean oxidation number of organic carbons, elemental composition, biomethane, theoretical biochemical methane potential, Buswell's ratio, biogas ratio, methane content percentage

1. Introduction

Anaerobic digestion (AD) is a sequence of bacteria-mediated biochemical processes and technologies (Batstone et al., 2002; Angelidaki & Sanders, 2004; Bidlingmaier, 2016; Banks, 2020). It is widely used for waste management, bioenergy production, and sustainable development (Horan et al., 2019; Holden et al., 2021; Torales, 2013). It is a cost-effective alternative to aerobic digestion, and has advantages in energy saving, reduction of sludge yield, and production of biofuel (Fang, 2010).

Buswell (Buswell & Boruff, 1932; Buswell & Hatfield, 1936; Buswell & Mueller, 1952) established the overall molecular chemical equation to represent organic matter in terms of their elemental composition regarding AD. An example of an unbalanced Buswell's equation (Symons & Buswell, 1933; Boyle, 1977) is shown below:

$$C_xH_yO_zN_vS_u + H_2O \rightarrow CH_4 + CO_2 + NH_3 + H_2S$$

The Buswell's equation is a model to quantify biomethane and the biochemical methane potential is a critical measuring parameter in AD (Holliger et al., 2016; Rodrigues et al., 2019; Yasim & Buyong, 2023; Koch et al., 2019).

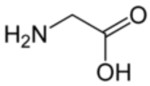
AD has been given less attention than aerobic digestion in biochemistry textbooks (Shen & Chen, 2021) and BEq is rarely mentioned in physical sciences and life sciences. Many students are unable to understand and manipulate the stoichiometric BEq. Although the concept of mean oxidation number of organic carbons has been applied in organic chemistry and biochemistry (Hanson, 1990; Halkides, 2000; Bentley et al., 2002; Yuen & Lau, 2022a), environmental chemistry (Kroll et al., 2011), biogeochemistry (Masiello et al., 2008; LaRowe & Van Cappellen, 2011; Dick et al., 2019), water treatment (Vogel et al., 2000), and organic combustion reaction (Yuen & Lau, 2023a), the relationship between ON_C and nCH_4 has not been studied.

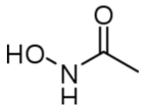
The purpose of this article is to explore the BEq model which can help unpack the redox nature of organic compounds and establish the mathematical relationship between mean oxidation number of organic carbons (ON_C) and theoretical quantity of biomethane (nCH_4). The H-atom method is used for balancing and deducting BEqs (Yuen & Lau, 2023b). The mathematical equation between ON_C and nCH_4 is then derived. Lastly, the Buswell's ratio, biogas ratio, biomethane content percentage, and theoretical biochemical methane potential (TBMP) can be calculated by using ON_C as a metric for any given organic compound.

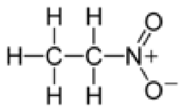
2. Procedures for Counting ON_N, ON_C, and Balancing BEq

Organonitrogen compounds are rich in nature and nitrogen is an essential element in life (Bada, 1998). The general formula of organonitrogen compound, $C_xH_yO_zN_v$, is chosen to be the model molecule for balancing and deducting BEqs.

The chemical formula of $C_2H_5O_2N$ has different isomers. Three of them are selected and shown as follows:

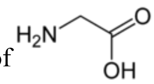


, 

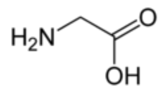
, and 

. They have different ON_N. The working procedure for assigning ON_N, ON_C, and balancing BEq is shown in Example 1.

Example 1. Establishing the balanced Buswell's equation (BEq) of $C_2H_5O_2N$

Step 1. Choose the structural formula of 

as the reactant

Count individual oxidation number (ON) of non-carbon atoms (Yuen & Lau, 2022a) for 

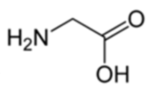
:

all hydrogen atoms: $ON_H = +1$

all oxygen atoms: $ON_O = -2$

one nitrogen atom: $ON_N = -3$

Step 2. Set up the BEq

The ON_N of the reactant (

) is identified as −3. The NH_3 ($ON_N = -3$) is selected to be the N-product accordingly.

The unbalanced BEq is shown as: $C_2H_5O_2N+H_2O \rightarrow CH_4+CO_2+NH_3$

Step 3. Balance the BEq by using the H-atom method (Yuen & Lau, 2021; 2022b)

Step 3.1 Divide an overall equation into two half reactions

$C_2H_5O_2N \rightarrow CH_4+NH_3$

$C_2H_5O_2N \rightarrow CO_2+NH_3$

Step 3.2 Balance two half reactions (from C→N→O→H)

$C_2H_5O_2N \rightarrow CH_4+NH_3$

$C_2H_5O_2N \rightarrow 2CH_4+NH_3$

$C_2H_5O_2N \rightarrow 2CH_4+NH_3+2O$

$C_2H_5O_2N+6H \rightarrow 2CH_4+NH_3+2O$

$C_2H_5O_2N+6H+4H \rightarrow 2CH_4+NH_3+2O+4H$

$C_2H_5O_2N+10H \rightarrow 2CH_4+NH_3+2H_2O$

$C_2H_5O_2N \rightarrow CO_2+NH_3$

$C_2H_5O_2N \rightarrow 2CO_2+NH_3$

$C_2H_5O_2N+2O \rightarrow 2CO_2+NH_3$

$C_2H_5O_2N+2O \rightarrow 2CO_2+NH_3+2H$

$C_2H_5O_2N+2O+4H \rightarrow 2CO_2+NH_3+2H+4H$

$C_2H_5O_2N+2H_2O \rightarrow 2CO_2+NH_3+6H$

Step 3.3 Combine two half reactions with equivalence of H-atom (LCM = 30)

$$(C_2H_5O_2N+10H\rightarrow 2CH_4+NH_3+2H_2O) \times 3$$

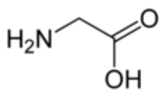
$$(C_2H_5O_2N+2H_2O\rightarrow 2CO_2+NH_3+6H) \times 5$$

$$8C_2H_5O_2N+4H_2O\rightarrow 6CH_4+10CO_2+8NH_3$$

$$C_2H_5O_2N+\frac{1}{2}H_2O\rightarrow \frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$$

Step 4. Identify the stoichiometric coefficients of nH_2O, nCH_4, and nCO_2

The stochiometric coefficients of $nH_2O = \frac{1}{2}$, $nCH_4 = \frac{3}{4}$, and $nCO_2 = \frac{5}{4}$ can be identified by the balanced BEq.

Step 5. Count the ON_C of 

By using the molecular formula method (IUPAC, 2019): $\Sigma ON_i = 0$

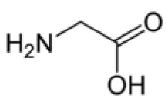
$$2ON_C + 5ON_H + 2ON_O + 1ON_N = 0$$

$$2ON_C = -5ON_H - 2ON_O - 1ON_N$$

$$\because ON_H = +1;\ ON_O = -2;\ ON_N = -3$$

$$\therefore 2ON_C = -5(+1) - 2(-2) - 1(-3)$$

$$ON_C = \frac{-5+4+3}{2} = +1$$

The ON_C of  ($C_2H_5O_2N$) equals +1.

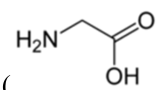
3. Relationships among ON_N, ON_C, and Stoichiometric Coefficients of $C_2H_5O_2N$ Molecules in BEq

By using the same procedure shown in Example 1 ($ON_N = -3$), different N-products are assigned by different ON_N. Nitrogen atoms have nine individual oxidation numbers (ON_N) and their values lie between the integer range of −3 to +5. The chemical formulas of N-products are combined with H-atom, O-atom, or both O-atom and H-atom. The resulting oxidation numbers of ON_N and ON_C, stoichiometric coefficients of nH_2O, nCH_4, and nCO_2 are summarized in Table 1. When the value of nH_2O is positive, it is on the reactant's side. When the value is negative, it is on the product's side.

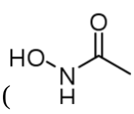
Table 1. Parameters of $C_2H_5O_2N$ molecules in the balanced BEqs

Equation #	Balanced Buswell's equation	ON_N	nH_2O	nCH_4	nCO_2	ON_C
1	$C_2H_5O_2N+\frac{1}{2}H_2O\rightarrow\frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$	−3	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{5}{4}$	+1
2	$C_2H_5O_2N+\frac{1}{4}H_2O\rightarrow\frac{7}{8}CH_4+\frac{9}{8}CO_2+\frac{1}{2}N_2H_4$	−2	$\frac{1}{4}$	$\frac{7}{8}$	$\frac{9}{8}$	$+\frac{1}{2}$
3	$C_2H_5O_2N\rightarrow CH_4+CO_2+\frac{1}{2}N_2H_2$	−1	0	1	1	0
4	$C_2H_5O_2N+H_2O\rightarrow CH_4+CO_2+NH_2OH$	−1	1	1	1	0
5	$C_2H_5O_2N\rightarrow\frac{9}{8}CH_4+\frac{7}{8}CO_2+\frac{1}{2}N_2+\frac{1}{4}H_2O$	0	$-\frac{1}{4}$	$\frac{9}{8}$	$\frac{7}{8}$	$-\frac{1}{2}$
6	$C_2H_5O_2N\rightarrow\frac{5}{4}CH_4+\frac{3}{4}CO_2+\frac{1}{2}N_2O+\frac{1}{2}H_2O$	+1	$-\frac{1}{2}$	$\frac{5}{4}$	$\frac{3}{4}$	−1
7	$C_2H_5O_2N\rightarrow\frac{11}{8}CH_4+\frac{5}{8}CO_2+NO+\frac{3}{4}H_2O$	+2	$-\frac{3}{4}$	$\frac{11}{8}$	$\frac{5}{8}$	$-\frac{3}{2}$
8	$C_2H_5O_2N+H_2O\rightarrow\frac{3}{2}CH_4+\frac{1}{2}CO_2+HNO_2$	+3	1	$\frac{3}{2}$	$\frac{1}{2}$	−2
9	$C_2H_5O_2N+\frac{1}{2}H_2O\rightarrow\frac{3}{2}CH_4+\frac{1}{2}CO_2+\frac{1}{2}N_2O_3$	+3	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{1}{2}$	−2
10	$C_2H_5O_2N\rightarrow\frac{13}{8}CH_4+\frac{3}{8}CO_2+\frac{1}{2}NO_2+\frac{5}{4}H_2O$	+4	$-\frac{5}{4}$	$\frac{13}{8}$	$\frac{3}{8}$	$-\frac{5}{2}$
11	$C_2H_5O_2N\rightarrow\frac{7}{4}CH_4+\frac{1}{4}CO_2+HNO_3+\frac{3}{2}H_2O$	+5	$-\frac{3}{2}$	$\frac{7}{4}$	$\frac{1}{4}$	−3
12	$C_2H_5O_2N+H_2O\rightarrow\frac{7}{4}CH_4+\frac{1}{4}CO_2+\frac{1}{2}N_2O_5$	+5	1	$\frac{7}{4}$	$\frac{1}{4}$	−3

With reference to Table 1, when Equation 1 and Equation 3 are compared, NH_3 ($ON_N = -3$) and N_2H_2 ($ON_N = -1$) have different ON_N, and their ON_C are +1 and 0 respectively. Consequently, they produce different stoichiometric coefficients of nCH_4 and nCO_2.

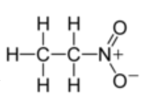
Equation 1: (

, ON_N = -3) $C_2H_5O_2N+\frac{1}{2}H_2O\rightarrow\frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$ ($ON_N = -3$)

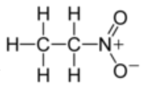
Equation 3: (

, ON_N = -1) $C_2H_5O_2N\rightarrow CH_4+CO_2+\frac{1}{2}N_2H_2$ ($ON_N = -1$)

When Equation 8 and Equation 9 are compared, N-products of HNO_2 and N_2O_3 have identical ON_N but different chemical formulas. Their ON_N produce the same ON_C of −2. Their stoichiometric coefficients of nCH_4 and nCO_2 remain the same in Equations 8 and 9.

Equation 8: (

, ON_N = +3) $C_2H_5O_2N+H_2O\rightarrow\frac{3}{2}CH_4+\frac{1}{2}CO_2+HNO_2$ ($ON_N = +3$)

Equation 9: ( , $ON_N = +3$) $C_2H_5O_2N+\frac{1}{2}H_2O\rightarrow\frac{3}{2}CH_4+\frac{1}{2}CO_2+\frac{1}{2}N_2O_3$ ($ON_N = +3$)

BEq is a biochemical redox reaction, in which the carbon atoms of an organic molecule disproportionate to CH_4 and CO_2. An ideal BEq model indicates that electron transfer occurs in sole organic carbons of organic compound, and other non-carbon atoms are not involved in the redox process.

4. Deducting the General BEq of $C_xH_yO_zN_v$ Molecules

NH_3 ($ON_N = -3$) is chosen as a N-product to balance BEq of $C_xH_yO_zN_v$ in Example 2.

Example 2. Deducting the BEq reaction of $C_xH_yO_zN_v$

Step 1. Set up the BEq reaction by choosing [N-product] ($ON_N = -3$)

$$C_xH_yO_zN_v+H_2O\rightarrow CH_4+CO_2+NH_3$$

Step 2. Deduct the BEq by using the H-atom method

Step 2.1 Divide an overall equation into two half reactions

$$C_xH_yO_zN_v\rightarrow CH_4+NH_3$$

$$C_xH_yO_zN_v\rightarrow CO_2+NH_3$$

Step 2.2 Balance two half reactions

$$C_xH_yO_zN_v\rightarrow xCH_4+vNH_3$$

$$C_xH_yO_zN_v+(4x-y+3v+2z)H\rightarrow vCH_4+vNH_3+zH_2O$$

$$C_xH_yO_zN_v\rightarrow xCO_2+vNH_3$$

$$C_xH_yO_zN_v+(2x-z)H_2O\rightarrow xCO_2+vNH_3+(4x+y-2z-3v)H$$

Step 2.3 Combine two half reactions with equivalence of H-atom {LCM=(4x−y+3v+2z) (4x+y−2z−3v)}

$$(C_xH_yO_zN_v+(4x-y+3v+2z)H\rightarrow vCH_4+vNH_3+zH_2O) \times (4x+y-2z-3v)$$

$$(C_xH_yO_zN_v+(2x-z)H_2O\rightarrow xCO_2+vNH_3+(4x+y-2z-3v)H) \times (4x-y+3v+2z)$$

$$8xC_xH_yO_zN_v+2x(4x-y-2z+3v)H_2O\rightarrow x(4x+y-2z-3v)CH_4+x(4x-y+2z+3v)CO_2+vNH_3$$

$$C_xH_yO_zN_v+\frac{4x-y-2z+3v}{4}H_2O\rightarrow\frac{4x+y-2z-3v}{8}CH_4+\frac{4x-y+2z+3v}{8}CO_2+vNH_3$$

Step 3. Identify the stoichiometric coefficients of nH_2O, nCH_4, and nCO_2

By using the atomic coefficients (AC) of the chemical formula, the stochiometric coefficients (SC) can be represented as follows: For [N-product] = NH_3 ($ON_N = -3$)

$$nCH_4 = \frac{4x+y-2z-3v}{8}$$

$$nCO_2 = \frac{4x-y+2z+3v}{8}$$

$$nH_2O = \frac{4x-y-2z+3v}{4}$$

Step 4. Count the ON_C

Count ON of non-carbon atoms:

all hydrogen atoms: $ON_H = +1$

all oxygen atoms: $ON_O = -2$

one nitrogen atom: $ON_N = -3$

By using the molecular formula method: $\Sigma ON_i = 0$

$$xON_C + y - 2z - 3v = 0$$

$$xON_C = -y + 2z + 3v$$

$$ON_C = \frac{-y+2z+3v}{x}$$

The ON_C of $C_xH_yO_zN_v$ is equal to $\frac{-y+2z+3v}{x}$.

4.1 Assigning Oxidation Numbers of ON_N and ON_C, and Balancing BEq for nH_2O, nCH_4, and nCO_2

By using the same procedure shown in Example 2, different N-products are assigned by different ON_N. The unbalanced BEq is shown as: $C_xH_yO_zN_v$+nH_2O H_2O→nCH_4 CH_4+nCO_2 CO_2+v[N-product]. Their ON_N, nH_2O, nCH_4, nCO_2, and ON_C are given in Table 2.

Table 2. Stoichiometric coefficients of nH_2O, nCH_4 and nCO_2, and oxidation numbers of ON_N, and ON_C in the balanced BEq of $C_xH_yO_zN_v$

ON_N of $C_xH_yO_zN_v$	nH_2O	nCH_4	nCO_2	ON_C	[N-product]
−3	$\frac{4x-y-2z+3v}{4}$	$\frac{4x+y-2z-3v}{8}$	$\frac{4x-y+2z+3v}{8}$	$\frac{-y+2z+3v}{x}$	NH_3
−2	$\frac{4x-y-2z+2v}{4}$	$\frac{4x+y-2z-2v}{8}$	$\frac{4x-y+2z+2v}{8}$	$\frac{-y+2z+2v}{x}$	N_2H_4
−1	$\frac{4x-y-2z+v}{4}$	$\frac{4x+y-2z-v}{8}$	$\frac{4x-y+2z+v}{8}$	$\frac{-y+2z+v}{x}$	N_2H_2
−1	$\frac{4x-y-2z+5v}{4}$	$\frac{4x+y-2z-v}{8}$	$\frac{4x-y+2z+v}{8}$	$\frac{-y+2z+v}{x}$	NH_2OH
0	$\frac{4x-y-2z}{4}$	$\frac{4x+y-2z}{8}$	$\frac{4x-y+2z}{8}$	$\frac{-y+2z}{x}$	N_2
+1	$\frac{4x-y-2z+v}{4}$	$\frac{4x+y-2z+v}{8}$	$\frac{4x-y+2z-v}{8}$	$\frac{-y+2z-v}{x}$	N_2O
+2	$\frac{4x-y-2z+2v}{4}$	$\frac{4x+y-2z+2v}{8}$	$\frac{4x-y+2z-2v}{8}$	$\frac{-y+2z-2v}{x}$	NO
+3	$\frac{4x-y-2z+3v}{4}$	$\frac{4x+y-2z+3v}{8}$	$\frac{4x-y+2z-3v}{8}$	$\frac{-y+2z-3v}{x}$	HNO_2
+3	$\frac{4x-y-2z+v}{4}$	$\frac{4x+y-2z+3v}{8}$	$\frac{4x-y+2z-3v}{8}$	$\frac{-y+2z-3v}{x}$	N_2O_3
+4	$\frac{4x-y-2z}{4}$	$\frac{4x+y-2z+4v}{8}$	$\frac{4x-y+2z-4v}{8}$	$\frac{-y+2z-4v}{x}$	NO_2
+5	$\frac{4x-y-2z+5v}{4}$	$\frac{4x+y-2z+5v}{8}$	$\frac{4x-y+2z-5v}{8}$	$\frac{-y+2z-5v}{x}$	HNO_3
+5	$\frac{4x-y-2z+7v}{4}$	$\frac{4x+y-2z+5v}{8}$	$\frac{4x-y+2z-5v}{8}$	$\frac{-y+2z-5v}{x}$	N_2O_5

By using the AC, the assigned ON of ON_H = +1, ON_O = −2, and ON_N, the SC of nCH_4, nCO_2, and ON_C can be represented as follows:

$$C_xH_yO_zN_v + nH_2O\ H_2O \rightarrow nCH_4\ CH_4 + nCO_2\ CO_2 + v[\text{N-product}]$$

$$nCH_4 = \frac{4x+y-2z+ON_N v}{8}$$

$$nCO_2 = \frac{4x-y+2z-ON_N\,v}{8}$$

$$ON_C = \frac{-y+2z-ON_N\,v}{x}$$

4.2 Mathematical Relationships among SC, AC, and ON of $C_xH_yO_zN_v$ Molecules

Any ON of non-carbon atoms (ON_H, ON_O, ON_N) and AC of $C_xH_yO_zN_v$ can be determined by its structural formula (Yuen & Lau, 2022a; 2023a).

ON of non-carbon atoms: ON_H, ON_O, ON_N

AC: x for carbon, y for hydrogen, z for oxygen, v for nitrogen

Atom	C	H	O	N
ON	-	ON_H	ON_O	ON_N
AC	x	y	z	v

The values of nCH_4, nCO_2, and ON_C can be calculated by using ON of ON_H, ON_O, and ON_N, and AC of x, y, z, and v.

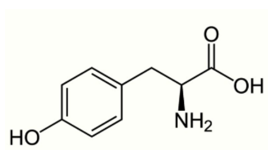
By balancing the BEq: $C_xH_yO_zN_v+H_2O \rightarrow CH_4+CO_2$+[H-product]+[O-product]+[N-product], the general derived mathematical equations of $C_xH_yO_zN_v$ molecules are given as follows:

$$nCH_4 = \frac{4x+ON_H\,y+ON_O\,z+ON_N\,v}{8}$$

$$nCO_2 = \frac{4x-ON_H\,y-ONO\,z-ON_N\,v}{8}$$

$$ON_C = \frac{-ON_H\,y-ON_O\,z-ON_N\,v}{x}$$

The value of ON for hydrogen is either −1 or +1, for oxygen it is either −1 or −2, and for nitrogen it is between the integer range of −3 to +5. By using the above derived general mathematical equations, the balanced BEq of $C_xH_yO_zN_v$ molecule can be found, and is shown in the following example.

Example 3. Given an example of tyrosine, 

, $C_9H_{11}O_3N$

(a) Identify AC and ON of non-carbon atoms

Atom	C	H	O	N
ON	-	+1	−2	−3
AC	9	11	3	1

(b) Use mathematical equations for calculating nCH_4, nCO_2, and ON_C

nCH_4	$= \frac{4x+ON_H\,y+ON_O\,z+ON_N\,v}{8}$	$= \frac{4(9)+(1)(11)-(2)(3)+(-3)(1)}{8} = \frac{19}{4}$
nCO_2	$= \frac{4x-ON_H\,y-ON_O\,z-ON_N\,v}{8}$	$= \frac{4(9)-(1)(11)+(2)(3)-(-3)(1)}{8} = \frac{17}{4}$
ON_C	$= \frac{-ON_H\,y-ON_O\,z-ON_N\,v}{x}$	$= \frac{-(1)(11)+2(3)-(-3)(1)}{9} = -\frac{2}{9}$

(c) Balance BEq by counting nH_2O

$$C_9H_{11}O_3N+nH_2O\ H_2O\rightarrow nCH_4\ CH_4+nCO_2\ CO_2+NH_3$$

$$C_9H_{11}O_3N+nH_2O\ H_2O\rightarrow \frac{19}{4}CH_4+\frac{17}{4}CO_2+NH_3$$

Balance O atom: $3 + nH_2O = \frac{17}{2}$

$$nH_2O = \frac{11}{2}$$

Balanced BEq: $C_9H_{11}O_3N+\frac{11}{2}H_2O\rightarrow \frac{19}{4}CH_4+\frac{17}{4}CO_2+NH_3$

5. Mathematical Relationships among nCH_4, nCO_2, and ON_C in $C_xH_yO_zX_wN_vS_uP_t$ Molecule

The strategy, which is used for balancing and deducting $C_xH_yO_zN_v$, can be extended to work on organic molecules containing the molecular formula $C_xH_yO_zX_wN_vS_uP_t$ (C, H, O, X, N, S, P stand for carbon, hydrogen, oxygen, halogen, nitrogen, sulfur, and phosphorus element respectively, and x, y, z, w, v, u, t stand for their corresponding atomic coefficients). For $C_xH_yO_zX_wN_vS_uP_t$, all possible ON of non-carbon atoms are shown as: $ON_H = +1$ or -1, $ON_O = -1$ or -2, ON_X = integer between -1 and $+7$, ON_N = integer between -3 and $+5$, ON_S = integer between -2 and $+6$, and ON_P = integer between -3 and $+5$.

The general unbalanced BEq is shown as:

$$C_xH_yO_zX_wN_vS_uP_t+H_2O\rightarrow CH_4+CO_2+[\text{H-product}]+[\text{O-product}]+[\text{X-product}]+[\text{N-product}]+[\text{S-product}]+[\text{P-product}].$$

The ON of non-carbon atoms and AC for calculating nCH_4, nCO_2, and ON_C are shown as follows:

Atom	C	H	O	X	N	S	P
ON	-	ON_H	ON_O	ON_X	ON_N	ON_S	ON_P
AC	x	y	z	w	v	u	t

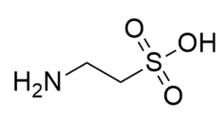
The derived general mathematical equations for $C_xH_yO_zX_wN_vS_uP_t$ are shown as follows:

$$nCH_4 = \frac{4x+ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t}{8}$$

$$nCO_2 = \frac{4x-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{8}$$

$$ON_C = \frac{-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{x}$$

By using these derived general mathematical equations, the balanced BEqs can be found by given structural formulas in Examples 4 to 7.

Example 4. Given an example of taurine, 

, $C_2H_7O_3NS$

(a) Identify AC and ON of non-carbon atoms

Atom	C	H	O	N	S
ON	-	+1	−2	−3	+4
AC	2	7	3	1	1

(b) Use mathematical equations to calculate nCH_4, nCO_2, and ON_C

Unbalanced BEq: $C_2H_7O_3NS+H_2O \rightarrow CH_4+CO_2+NH_3+SO_2$

nCH_4	$= \frac{4x+ON_H y+ON_O z+ON_N v+ON_S u}{8}$	$= \frac{4(2)+(1)(7)+(-2)(3)+(-3)(1)+(+4)(1)}{8} = \frac{5}{4}$
nCO_2	$= \frac{4x-ON_H y-ON_O z-ON_N v-ON_S u}{8}$	$= \frac{4(2)-(1)(7)-(-2)(3)-(-3)(1)-(+4)(1)}{8} = \frac{3}{4}$
ON_C	$= \frac{-ON_H y-ON_O z-ON_N v-ON_S u}{x}$	$= \frac{-(1)(7)-(-2)(3)-(-3)(1)-(+4)(1)}{2} = -1$

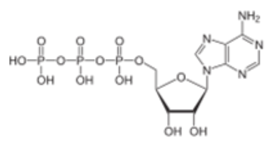
(c) Balance BEq by counting nH_2O

$$C_2H_7O_3NS+nH_2O\ H_2O \rightarrow \frac{5}{4}CH_4+\frac{3}{4}CO_2+NH_3+SO_2$$

Balance O atom: $3 + nH_2O = \frac{3}{2} + 2$

$$nH_2O = \frac{1}{2}$$

Attained balanced BEq: $C_2H_7O_3NS+\frac{1}{2}H_2O \rightarrow \frac{5}{4}CH_4+\frac{3}{4}CO_2+NH_3+SO_2$

Example 5. Balancing the Buswell's equation for ATP,  , $C_{10}H_{16}O_{13}N_5P_3$

(a) Identify AC and ON of non-carbon atoms

Atom	C	H	O	N	P
ON	-	+1	−2	−3	+5
AC	10	16	13	5	3

(b) Use mathematical equations to calculate nCH_4, nCO_2, and ON_C

Unbalanced BEq: $C_{10}H_{16}O_{13}N_5P_3+H_2O \rightarrow CH_4+CO_2+NH_3+H_3PO_4$

nCH_4	$= \frac{4x+ON_H y+ON_O z+ON_N v+ON_P t}{8}$	$= \frac{4(10)+(1)(16)+(-2)(13)+(-3)(5)+(+5)(3)}{8} = \frac{15}{4}$
nCO_2	$= \frac{4x-ON_H y-ON_O z-ON_N v-ON_P t}{8}$	$= \frac{4(10)-(1)(16)-(-2)(13)-(-3)(5)-(+5)(3)}{8} = \frac{25}{4}$
ON_C	$= \frac{-ON_H y-ON_O z-ON_N v-ON_P t}{x}$	$= \frac{-(1)(16)-(-2)(13)-(-3)(5)-(+5)(3)}{10} = +1$

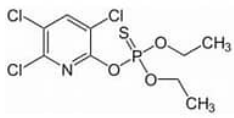
(c) Balance BEq by counting nH_2O

$$C_{10}H_{16}O_{13}N_5P_3+nH_2O\ H_2O \rightarrow \frac{15}{4}CH_4+\frac{25}{4}CO_2+5NH_3+3H_3PO_4$$

Balance O atom: $13 + nH_2O = \frac{25}{2} + 12$

$$nH_2O = \frac{23}{2}$$

Attained balanced BEq: $C_{10}H_{16}O_{13}N_5P_3+\frac{23}{2}H_2O \rightarrow \frac{15}{4}CH_4+\frac{25}{4}CO_2+5NH_3+3H_3PO_4$

Example 6. Given chlorpyrifos, 

, $C_9H_{11}O_3Cl_3NSP$

(a) Identify AC and ON of non-carbon atoms

Atom	C	H	O	Cl	N	S	P
ON	-	+1	−2	−1	−3	−2	+5
AC	9	11	3	3	1	1	1

(b) Use mathematical equations to calculate nCH_4, nCO_2, and ON_C

Unbalanced BEq: $C_9H_{11}O_3Cl_3NSP+H_2O \rightarrow CH_4+CO_2+HCl+NH_3+H_2S+H_3PO_4$

nCH_4	$= \frac{4x+ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t}{8}$	$= \frac{4(9)+(1)(11)+(-2)(3)+(-1)(3)+(-3)(1)+(-2)(1)+(+5)(1)}{8} = \frac{19}{4}$
nCO_2	$= \frac{4x-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{8}$	$= \frac{4(9)-(1)(11)-(-2)(3)-(-1)(3)-(-3)(1)-(-2)(1)-(+5)(1)}{8} = \frac{17}{4}$
ON_C	$= \frac{-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{x}$	$= \frac{-(1)(11)-(-2)(3)-(-1)(3)-(-3)(1)-(-2)(1)-(+5)(1)}{9} = -\frac{2}{9}$

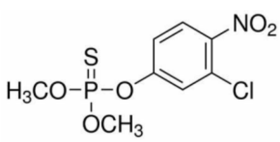
(c) Balance BEq by counting nH_2O

$$C_9H_{11}O_3Cl_3NSP+nH_2O\ H_2O \rightarrow \frac{19}{4}CH_4+\frac{17}{4}CO_2+3HCl+NH_3+H_2S+H_3PO_4$$

Balance O atom: $3 + nH_2O = \frac{17}{2} + 4$

$$nH_2O = \frac{19}{2}$$

Attained balanced BEq: $C_9H_{11}O_3Cl_3NSP+\frac{19}{2}H_2O \rightarrow \frac{19}{4}CH_4+\frac{17}{4}CO_2+3HCl+NH_3+H_2S+H_3PO_4$

Example 7. Given chlorthion, 

, $C_8H_9O_5ClNPS$

(a) Identify AC and ON of non-carbon atoms

Atom	C	H	O	Cl	N	S	P
ON	-	+1	−2	−1	+3	−2	+5
AC	8	9	5	1	1	1	1

(b) Use mathematical equations to calculate nCH_4, nCO_2, and ON_C

Unbalanced BEq: $C_8H_9O_5ClNPS+H_2O \rightarrow CH_4+CO_2+HCl+HNO_2+H_2S+H_3PO_4$

nCH_4	$= \frac{4x+ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t}{8}$	$= \frac{4(8)+(1)(9)+(-2)(5)+(-1)(1)+(+3)(1)+(-2)(1)+(+5)(1)}{8} = \frac{9}{2}$
nCO_2	$= \frac{4x-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{8}$	$= \frac{4(8)-(1)(9)-(-2)(5)-(-1)(1)-(+3)(1)-(-2)(1)-(+5)(1)}{8} = \frac{7}{2}$
ON_C	$= \frac{-ON_H\,y-ON_O\,z-ON_X\,w-ON_N\,v-ON_S\,u-ON_P\,t}{x}$	$= \frac{-(1)(9)-(-2)(5)-(-1)(1)-(+3)(1)-(-2)(1)-(+5)(1)}{8} = -\frac{1}{2}$

(c) Balance BEq by counting nH_2O

$$C_8H_9O_5ClNPS+nH_2O\ H_2O\rightarrow\frac{9}{2}CH_4+\frac{7}{2}CO_2+HCl+HNO_2+H_2S+H_3PO_4$$

Balance O atom: $5 + nH_2O = 7 + 2 + 4$

$nH_2O = 8$

Attained balanced BEq: $C_8H_9O_5ClNPS+8H_2O\rightarrow\frac{9}{2}CH_4+\frac{7}{2}CO_2+HCl+HNO_2+H_2S+H_3PO_4$

6. Mathematical Relationship between ONc and nCH_4

Based on the following mathematical equations,

$$x = n_C = nCH_4 + nCO_2$$

$$ON_C = \frac{-ON_H\ y-ON_O\ z-ON_X\ w-ON_N\ v-ON_S\ u-ON_P\ t}{x}$$

$$nCH_4 = \frac{4x+ON_H\ y+ON_O\ z+ON_X\ w+ON_N\ v+ON_S\ u+ON_P\ t}{8}$$

$$nCO_2 = \frac{4x-ON_H\ y-ON_O\ z-ON_X\ w-ON_N\ v-ON_S\ u-ON_P\ t}{8}$$

new mathematical equations can be derived as follows:

$$\because x\ ON_C = -ON_H\ y - ON_O\ z - ON_X\ w - ON_N\ v - ON_S\ u - ON_P\ t$$

$$\therefore nCH_4 = \frac{x(4-ON_C)}{8} \text{ and } nCO_2 = \frac{x(4+ON_C)}{8}$$

Consequently, the important parameters of BEq, which include Buswell's ratio ($\frac{nCH_4}{nCO_2}$), biogas ratio ($\frac{nCH_4}{nCH_4+nCO_2}$), methane content percentage ($\frac{nCH_4}{nCH_4+nCO_2}\times100\%$), and TBMP ($\frac{x(4-ON_C)(22400)}{8\mu}$) can be determined by using the sole ON_C , or ON_C to complement x and/or μ. These parameters and their mathematical equations are summarized in Table 3.

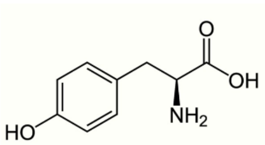
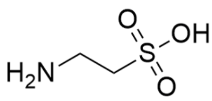
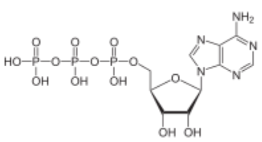
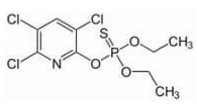
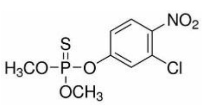
Table 3. Mathematical equations for parameters of BEq and ON_C

Parameter of BEq	Mathematical equation	
nCH_4	$= \frac{4x+ON_H\ y+ON_O\ z+ON_X\ w+ON_N\ v+ON_S\ u+ON_P\ t}{8}$	$= \frac{x(4-ON_C)}{8}$
nCO_2	$= \frac{4x-ON_H\ y-ON_O\ z-ON_X\ w-ON_N\ v-ON_S\ u-ON_P\ t}{8}$	$= \frac{x(4+ON_C)}{8}$
Buswell's ratio	$= \frac{nCH_4}{nCO_2}$	$= \frac{(4-ON_C)}{(4+ON_C)}$
Biogas* ratio	$= \frac{nCH_4}{nCH_4+nCO_2}$	$= \frac{(4-ON_C)}{8}$
Methane content percentage (nCH_4 %)	$= \frac{nCH_4}{nCH_4+nCO_2} \times 100\%$	$= \frac{(4-ON_C)}{8}\times100\%$
TBMP (at STP, mL/g)	$= \frac{22400(nCH_4)}{\mu}$	$= \frac{x(4-ON_C)(22400)}{8\mu}$

*Biogas is defined as the sum of quantitative amounts of biomethane and carbon dioxide ($n_{biogas} = nCH_4 + nCO_2$).

When ON_C for any given molecule is determined, the parameters of BEq can be counted. According to the molecules in Examples 3 – 7, all the resulting values of parameters of BEq are exhibited in Table 4.

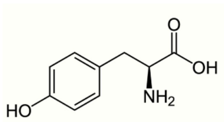
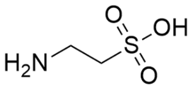
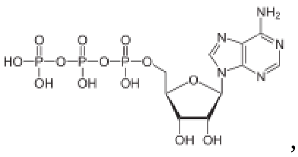
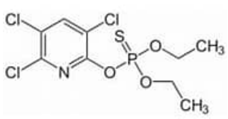
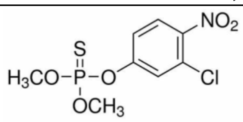
Table 4. ON_C for determination of nCH_4, nCO_2, and parameters of BEq

Molecule	ON_C	x	$nCH_4 = \frac{x(4-ON_C)}{8}$	$nCO_2 = \frac{x(4+ON_C)}{8}$	Buswell's ratio $= \frac{(4-ON_C)}{(4+ON_C)}$	Biogas ratio $= \frac{(4-ON_C)}{8}$	nCH_4 % $= \frac{(4-ON_C)}{8} \times 100\%$
 , $C_9H_{11}O_3N$	$-\frac{2}{9}$	9	$\frac{19}{4}$	$\frac{17}{4}$	$\frac{19}{17} = 1.12$	$\frac{19}{36} = 0.53$	52.78%
 , $C_2H_7O_3NS$	−1	2	$\frac{5}{4}$	$\frac{3}{4}$	$\frac{5}{3} = 1.67$	$\frac{5}{8} = 0.63$	62.50%
 , $C_{10}H_{16}O_{13}N_5P_3$	+1	10	$\frac{15}{4}$	$\frac{25}{4}$	$\frac{3}{5} = 0.60$	$\frac{3}{8} = 0.38$	37.50%
 , $C_9H_{11}O_3Cl_3NSP$	$-\frac{2}{9}$	9	$\frac{19}{4}$	$\frac{17}{4}$	$\frac{19}{17} = 1.12$	$\frac{19}{36} = 0.53$	52.78%
 , $C_8H_9O_5ClNPS$	$-\frac{1}{2}$	8	$\frac{9}{2}$	$\frac{7}{2}$	$\frac{9}{7} = 1.29$	$\frac{9}{16} = 0.56$	56.25%

With reference to the results in Table 4, Buswell's ratio, biogas ratio, and methane content percentage are determined by the assigned ON_C of a given molecule. The nCH_4 and nCO_2 can be counted by ON_C and its number of organic carbons (x).

According to the given molecules in Examples 3 − 7, all resulting values are summarized in Table 5. The TBMP can be calculated by ON_C, x, and molecular mass (μ) for any given organic molecule.

Table 5. Counting TBMP by ON_C, x, and μ

Molecule	ON_C	x	Molecular mass (μ) (g/mol)	TBMP = $\frac{x(4-ON_C)(22400)}{8\mu}$ (mL/g)
 , $C_9H_{11}O_3N$	$-\frac{2}{9}$	9	181.19	587.23
 , $C_2H_7O_3NS$	−1	2	125.15	223.73
 , $C_{10}H_{16}O_{13}N_5P_3$	+1	10	240.97	348.59
 , $C_9H_{11}O_3Cl_3NSP$	$-\frac{2}{9}$	9	350.59	303.49
 , $C_8H_9O_5ClNPS$	$-\frac{1}{2}$	8	297.65	338.65

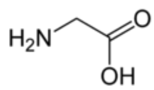
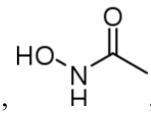
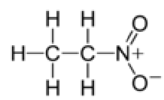
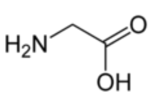
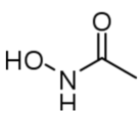
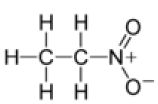
With reference to Table 1, three structural formulas of $C_2H_5O_2N$ are  ,  , and  . Their ON_C values are +1, 0, and −2 respectively. All parameters of BEq are calculated and summarized in Table 6. Among these isomers of $C_2H_5O_2N$, the isomer carrying the highest reduced ON_C can produce the most TBMP.

Table 6. ONc for determination of nCH_4, nCO_2, and BEq's parameters for $C_2H_5O_2N$ molecules

$C_2H_5O_2N$ Molecule x =2 μ = 75.07 g/mol	ON_N	ON_C	nCH_4 = $\frac{x(4-ON_C)}{8}$	nCO_2 = $\frac{x(4+ON_C)}{8}$	Buswell's ratio = $\frac{(4-ON_C)}{(4+ON_C)}$	Biogas ratio = $\frac{(4-ON_C)}{8}$	nCH_4 % = $\frac{(4-ON_C)}{8}$×100%	TBMP = $\frac{x(4-ON_C)(22400)}{8\mu}$ (mL/g)
	−3	+1	$\frac{3}{4}$	$\frac{5}{4}$	$\frac{3}{5}$	$\frac{3}{8}$	37.50%	223.79
	−1	0	1	1	1	$\frac{1}{2}$	50.00%	298.39
	+3	−2	$\frac{3}{2}$	$\frac{1}{2}$	3	$\frac{3}{4}$	75.00%	447.58

7. Conclusion

The ON_C is an important redox concept in organic chemistry and biochemistry. In this article, the BEq model is developed by using the H-atom method for understanding the redox nature of organic compounds. ON_C acts as a metric for quantifying parameters of BEq. The mathematical relationship between ON_C and nCH_4 is established as $nCH_4 = \frac{x(4-ON_C)}{8}$.

Consequently, for any given structural formula of an organic molecule, the parameters of BEq, such as quantity of biomethane, Buswell's ratio, biogas ratio, biomethane content percentage and theoretical biochemical methane potential can be determined.

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Authors contributions

Dr. Pong Kau Yuen was responsible for designing the study, drafting, and revising the manuscript. Dr. Cheng Man Diana Lau was responsible for revising the manuscript. All authors read and approved the final manuscript.

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The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Obtained.

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Data availability statement

The data that support the findings of this study are available on request from the corresponding author. The data is not publicly available due to privacy or ethical restrictions.

Data sharing statement

No additional data is available.

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