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Counting and Demonstrating Electron Transfer in Buswell's Equation

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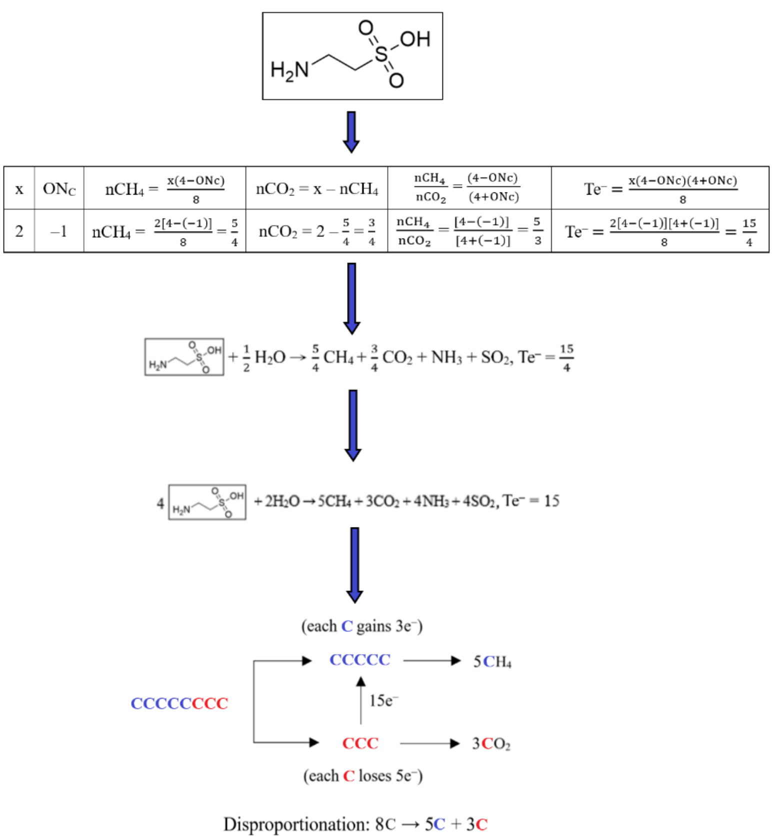
Abstract

Anaerobic digestion is a microorganism-mediated redox system chemically represented by Buswell's equation. In the equation, the quantity of methane and carbon dioxide can be counted by the elemental composition of organic matter; however, there is a lack of connection between electron transfer and formations of methane and carbon dioxide. Although the mechanism of direct interspecies and mediated interspecies electron transfer in anaerobic digestion has been widely researched, the method of counting electron transfer in Buswell's equation has not yet been explored. This article develops a method to count electron transfer of organic molecules in Buswell's equation. Mathematical equations are established through integration of relationships between mean oxidation number of organic carbons, quantity of methane, and number of transferred electrons. With any known organic structural formula, three tasks can be achieved: (1) determination of the Buswell-Ratio, (2) counting of Buswell-Electron, and (3) demonstration of electron transfer among organic carbons by drawing the Buswell-Electron diagram.

Graphical abstract



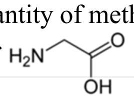
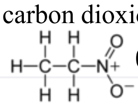
Keywords: anaerobic digestion, Buswell's equation, mean oxidation number of organic carbons, quantity of methane, number of transferred electrons, Buswell-Electron diagram

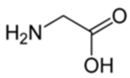
1. Introduction

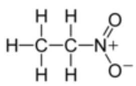
Anaerobic digestion (AD) is a natural activity and industrial biochemical technology (Meegoda et al., 2018; Náthia-Neves et al., 2018) in which organic matters are mineralized or stabilized by microorganisms in the absence of molecular oxygen. AD facilitates waste volume reduction, biofertilizer preparation, biofuel production (Torales, 2013; Horan et al., 2019), and biochemical syntheses (Bolzonella et al., 2023; Kusch-Brandt et al., 2023). However, it poses disadvantages of slow conversion rates and low conversion efficiencies to methane (Zhao et al., 2020). Buswell's equation (BEq*)* is established to represent AD chemically (Buswell & Mueller, 1952; Boyle, 1977). Based on the elemental composition of organic matter, the equation counts the quantity of biogas and digestates. The general balanced BEq for $C_xH_yO_zX_wN_vS_uP_t$ (Yuen & Lau, 2023a) is shown in the following:

$$C_xH_yO_zX_wN_vS_uP_t + \frac{4x-y-2z+w+3v+2u+11t}{4} H_2O \rightarrow \frac{4x+y-2z-w-3v-2u+5t}{8} CH_4 + \frac{4x-y+2z+w+3v+2u-5t}{8} CO_2 + wHX + vNH_3$$

$$+ uH_2S + tH_3PO_4.$$

BEq is a model that is represented by a stoichiometric chemical equation. It assumes that: (i) pure or mixed organic matter is represented by an empirical formula, (ii) water is involved in BEq, (iii) all carbon atoms convert totally to CH_4 and CO_2, and (iv) all heteroatoms (halogen, nitrogen, sulfur, and phosphorous) convert to HX, NH_3, H_2S, and H_3PO_4, respectively. The significance of quantity of methane (nCH_4) is to count theoretical biomethane potential (Angelidaki & Sanders, 2004). Organic molecules that have identical empirical formulas but different structural formulas will produce identical quantity of methane (nCH_4) and carbon dioxide (nCO_2). To illustrate this, two different stoichiometric chemical equations of  ($C_2H_5O_2N$) and  ($C_2H_5O_2N$) are shown in the following:

Eq1:  ($C_2H_5O_2N$) + $\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$

Eq2:  ($C_2H_5O_2N$) + $\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$

Using the mentioned BEq model, both Eq1 and Eq2 are BEq. This article addresses several questions: (1) Which equation is a BEq, Eq1, or Eq2? (2) Are they both BEq? (3) How can a BEq be identified? (4) What are the criteria to identify a BEq?

BEq is a well-known redox reaction, the nature of which is electron transfer. The mechanism of direct interspecies electron transfer (DIET) (Lovley, 2017; Feng et al., 2021; Feng et al., 2022; Chen et al., 2022) and mediated interspecies electron transfer (MIET) (Storck et al., 2016; Wang et al. 2023), such as interspecies hydrogen transfer (Yuan et al, 2021), interspecies formate transfer (Day et al., 2022), and interspecies redox carriers transfer (Smith et al., 2015; Palacios et al., 2023) have been proposed. Although the microorganisms-mediated electron transfer mechanism in AD has been widely researched (Rotaru et al., 2014; Lin, 2022; Su et al., 2024), the method of counting electron transfer in BEq has not yet been explored.

Oxidation number (ON) is a key redox concept for counting the number of transferred electrons (Te^-) (IUPAC, 1997). The mean oxidation number of organic carbons (ON_C) not only serves as a redox indicator of organic matter, but also a valuable redox metric for understanding organic carbon's characteristics. ON_C has many uses: assessing organic molecules in biochemical cycle (Hanson,1990), monitoring carbon cycle in ecosystem (Masiello et al. 2008), measuring organic quantity in wastewater (Vogel et al., 2000), following organic aerosols in atmosphere (Kroll et al., 2011), determining free energy changes of organic carbons in half oxidation reactions (LaRowe & Van Cappellen, 2011), assigning redox biomolecules in geochemistry (Dick & Shock, 2011), and counting oxidative ratio in organic combustion reactions (Yuen & Lau, 2023b). Although the mathematical relationship between ON_C and nCH_4 in BEq has already been established (Yuen & Lau, 2024a), there is still a conceptual void among ON_C, nCH_4, and Te^-. This article argues that when the redox nature of BEq can be interpreted by electron transfer among organic carbons, the criteria for identifying BEq can be developed. Consequently, the questions that were raised above can be answered.

Based on structural formulas of organic molecules, ON_C is a key redox parameter to explore the redox nature of BEq. The aims of this article are (i) to establish the relationships between ON_C, nCH_4, and Te^-, (ii) to develop a method for counting Te^- of organic molecules in BEq, and (iii) to establish a Buswell-Electron diagram (BEq-Te^- diagram) for demonstrating the involved Te^-.

2. Methods and Materials

2.1 Determination of Mean Oxidation Number of Organic Carbons (ON_C)

Based on the structural formula of an organic matter, the individual oxidation number of atoms (ON_i) can be assigned by the fragmentation method (Yuen & Lau, 2022a), and ON_C can be counted by the non-carbon atom method (Yuen & Lau, 2024b).

For organic matters: $C_xH_yO_zX_wN_vS_uP_t^{charge}$

C, H, O, X, N, S, P = carbon, hydrogen, oxygen, halogen, nitrogen, sulfur, and phosphorus elements

x, y, z, w, v, u, t = atomic coefficients for C, H, O, X, N, S, P

charge = electrical charge of organic matter

nc = x = number of organic carbons

ON_{inc} = individual oxidation number of non-carbon atoms

AC = atomic coefficients

When charge ≠ 0, $ON_C = \frac{\text{charge} - \Sigma ON_{inc}}{nc}$.

When charge = 0, $ON_C = \frac{-\Sigma ON_{inc}}{nc}$.

Given a structural formula of $C_xH_yO_zX_wN_vS_uP_t$

$C_xH_yO_zX_wN_vS_uP_t$	C	H	O	X	N	S	P
ON_{inc}	-	ON_H	ON_O	ON_X	ON_N	ON_S	ON_P
AC	x	y	z	w	v	u	t

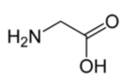
$\Sigma ON_{inc} = [(ON_H\ y) + (ON_O\ z) + (ON_X\ w) + (ON_N\ v) + (ON_S\ u) + (ON_P\ t)]$

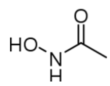
The mathematical equation for calculating ON_C is established for neutral organic molecules in their structural formulas:

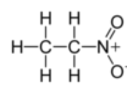
$$ON_C = \frac{-\Sigma ON_{inc}}{nc}$$

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

2.2 Isomers of Organonitrogen Molecules

The organonitrogen molecules, $C_xH_yO_zN_v$ and $C_2H_5O_2N$, are chosen to illustrate the counting of Te^- in BEq. Three selected structural formulas of $C_2H_5O_2N$ isomers are: 

, 

, and 

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An empirical formula shows the elemental composition only, and a structural formula identifies the covalent bond skeletal of all atoms. Based on the known structural formulas, the AC, ON_{inc}, and ON_C can be assigned and determined.

2.3 H-atom Method

The H-atom method is a half reaction-based approach in which H, O, and H_2O are balancing tools. It can be used to balance, deduce, quantify, and define redox reactions (Yuen & Lau, 2022b, 2023b). It can also be used to understand BEq (Yuen & Lau; 2024a).

2.4 Organic Redox Couples

In a balanced half organic redox reaction, any organic redox couple can be represented by the mathematical equation of $Te^- = nc\ \Delta ON_C$ (Yuen & Lau, 2022c). Changes in mean oxidation number of organic carbons (ΔON_C) of two organic redox couples in BEq are shown in the following:

$\Delta ON_{C1} = ON_C(CH_4) - ON_C$ (organic molecule)

$\Delta ON_{C2} = ON_C(CO_2) - ON_C$ (organic molecule)

2.5 Buswell's Equation (BEq)

When the empirical formulas of organic matter are given, the general balanced BEq for $C_xH_yO_zX_wN_vS_uP_t$ is as shown (Yuen & Lau, 2023a):

$$C_xH_yO_zX_wN_vS_uP_t + \frac{4x-y-2z+w+3v+2u+11t}{4} H_2O \rightarrow \frac{4x+y-2z-w-3v-2u+5t}{8} CH_4 + \frac{4x-y+2z+w+3v+2u-5t}{8} CO_2 + wHX + vNH_3 + uH_2S + tH_3PO_4$$

Based on the elemental composition, nCH_4, nCO_2, and $\frac{nCH_4}{nCO_2}$ can be determined by the following mathematical equations, respectively.

$nCH_4 = \frac{4x+y-2z-w-3v-2u+5t}{8}$	$nCO_2 = \frac{4x-y+2z+w+3v+2u-5t}{8}$	$\frac{nCH_4}{nCO_2} = \frac{4x+y-2z-w-3v-2u+5t}{4x-y+2z+w+3v+2u-5t}$

2.6 ON_C-Buswell's Equation (ON_C-BEq)

The general unbalanced BEq for $C_xH_yO_zX_wN_vS_uP_t$ (Yuen & Lau; 2024a) is shown as:

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

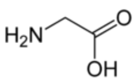
Based on any structural formula of an organic molecule, x, nCH_4, nCO_2, and $\frac{nCH_4}{nCO_2}$ can be determined by the following mathematical equations:

$x = nCH_4 + nCO_2$	$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = \frac{x(4+ONc)}{8}$	$\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$

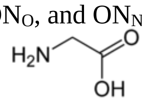
3. Procedures for Counting Electron Transfer in Buswell's Equation

To count Te^- in BEq, follow these three steps: (i) use the structural formula method to assign ON_i, (ii) use the H-atom method to balance BEq, and (iii) use the organic redox couple equation to count Te^-. The working scheme is shown as follows:

a structural formula → AC, ON_{inc}, and ON_C → stoichiometric coefficients (SC) → Te^-.

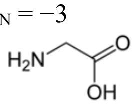
Example 1. Given a structural formula  ($C_2H_5O_2N$), count the Te^- in BEq.

Step 1. Assign ON_{inc} (ON_H, ON_O, and ON_N) and ON_C

Using fragmentation method,  → $H_2N^- + {}^+H_2CCOOH$

1.1 Count ON_{inc} of H_2N^-

$ON_H = +1$, $ON_N = -3$

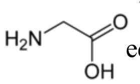
1.2 Count ON_C of 

Using the non-carbon atom method, ON_C can be counted by ON_{inc} and AC.

Atom	C	H	O	N
ON_{inc}	-	+1	−2	−3
AC	2	5	2	1

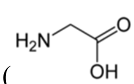
$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(ON_H\ y + ON_O\ z + ON_N\ v)}{x}$$

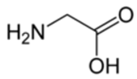
$$ON_C = \frac{-[(+1)5+(-2)2+(-3)1]}{2} = +1$$

The ON_C of  equals +1.

Step 2. Balance BEq

2.1 Set up the unbalanced BEq

The ON_N of the reactant () is identified as −3. The NH_3 ($ON_N = -3$) is selected as the designated N-product accordingly.

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

2.2 Balance BEq using the H-atom method

Divide an overall equation into two half reactions

$C_2H_5O_2N \rightarrow CH_4 + NH_3$

$C_2H_5O_2N \rightarrow CO_2 + NH_3$

Balance two half reactions

$C_2H_5O_2N \rightarrow CH_4 + NH_3$

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

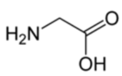
$C_2H_5O_2N \rightarrow CO_2 + NH_3$

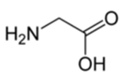
$C_2H_5O_2N + 2H_2O \rightarrow 2CO_2 + NH_3 + 6H$

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

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

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

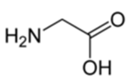
8  $+4H_2O \rightarrow 6CH_4 + 10CO_2 + 8NH_3$

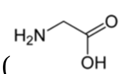
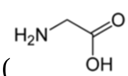
 $+\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$

The SC 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 3. Count Te^-

Using the equation of $Te^- = nc\ \Delta ON_C$ for organic redox couples, Te^- can be counted by the parameters ΔON_C, nCH_4, and nCO_2.

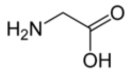
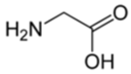
Based on the balanced BEq:  $+\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$, the Te^- (reduction) and Te^- (oxidation) on carbon atoms can be determined as follows:

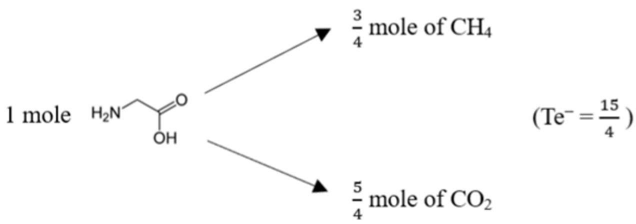
Reduction:	Oxidation:
$Te^- = nCH_4\ \Delta ON_{C1}$ $= nCH_4\ [ON_C\ (CH_4) - ON_C$ ()] $= nCH_4\ [(-4) - ON_C\ (C_2H_5O_2N)]$ $\because nCH_4 = \frac{3}{4}$; $ON_C\ (C_2H_5O_2N) = +1$ $\therefore Te^- = \frac{3}{4}\ [(-4) - (+1)]$ $= -\frac{15}{4}$ (a gain of $\frac{15}{4}$ electrons)	$Te^- = nCO_2\ \Delta ON_{C2}$ $= nCO_2\ [ON_C\ (CO_2) - ON_C$ ()] $= nCO_2\ [(+4) - ON_C\ (C_2H_5O_2N)]$ $\because nCO_2 = \frac{5}{4}$; $ON_C\ (C_2H_5O_2N) = +1$ $\therefore Te^- = \frac{5}{4}\ [(+4) - (+1)]$ $= +\frac{15}{4}$ (a loss of $\frac{15}{4}$ electrons)

The "−" represents a gain of electrons (half reduction reaction) and the "+" represents a loss of electrons (half oxidation reaction).

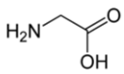
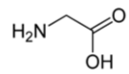
4. Demonstration of Electron Transfer in Buswell's Equation

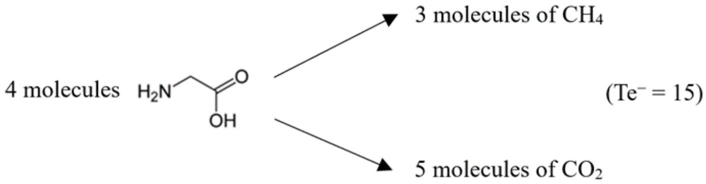
4.1 Description of Macro-BEq

The Macro-BEq is shown as:  $+\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$, $Te^- = \frac{15}{4}$. Macroscopically, 1 mole of  involves $\frac{15}{4}$ electrons disproportionate to $\frac{3}{4}$ mole of CH_4 and $\frac{5}{4}$ mole of CO_2.

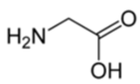
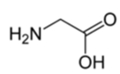


4.2 Description of Micro-BEq

Considering non-integer numbers of SC and Te^- in the Macro-BEq, by multiplying 4 the Micro-BEq can be generated and is shown as 4  $+2H_2O \rightarrow 3CH_4 + 5CO_2 + 4NH_3$, $Te^- = 15$. Microscopically, 4 molecules of  involve 15 electrons disproportionate to 3 molecules of CH_4 and 5 molecules of CO_2.



4.3 Demonstration of BEq-Te⁻ Diagram

In the structure of 4  molecules (8 carbon atoms), there are 3 carbon atoms, each of which gains 5 electrons (total gain of $15e^-$) to form 3 CH_4 molecules, and there are 5 other carbon atoms, each of which loses 3 electrons (total loss of $15e^-$) to form 5 CO_2 molecules. A BEq-Te^- diagram of 4  molecules (8 carbons) is shown in Figure 1.

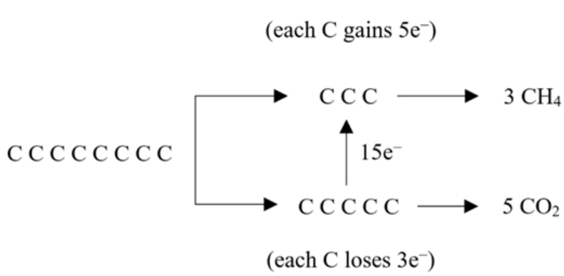
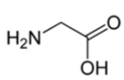


Figure 1. The BEq-Te^- diagram for  molecules

4.4 Interpretation of Te^-

ΣTe^- = net number of transferred electrons in overall redox reactions

$\Sigma Te^- = 0$

For $C_xH_yO_zN_v$ molecules,

$\Sigma Te^- = Te^-$ (C1 for CH_4) + Te^- (C2 for CO_2) + Te^- (H) + Te^- (O) + Te^- (N)

$\Sigma Te^- = nCH_4\ \Delta ON_{C1} + nCO_2\ \Delta ON_{C2} + n_H\ \Delta ON_H + n_O\ \Delta ON_O + n_N\ \Delta ON_N$

When all ON_{inc} remain the same before and after a redox reaction, $\Delta ON_H = 0$, $\Delta ON_O = 0$, and $\Delta ON_N = 0$ are attained. All non-carbon atoms are identified as non-redox atoms.

$0 = Te^-$ (C1 for CH_4) + Te^- (C2 for CO_2)

$0 = nCH_4\ \Delta ON_{C1}$ (gain of electrons) + $nCO_2\ \Delta ON_{C2}$ (loss of electrons)

$-nCH_4\ \Delta ON_{C1} = nCO_2\ \Delta ON_{C2}$

$-nCH_4\ (-4-ONc) = nCO_2\ (4-ONc)$

$nCH_4\ (4+ONc) = nCO_2\ (4-ONc)$

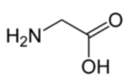
$$\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$$

Te^- (C1 for CH_4) means Te^- (reduction for CH_4).

Te^- (C2 for CO_2) means Te^- (oxidation for CO_2).

When Te^- (reduction for CH_4) = Te^- (oxidation for CO_2), the mathematical relation of $\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$ is established.

4.5 Disproportionation of Organic Carbons

All organic carbons are redox atoms. Since there is no gain or loss of electrons among non-carbon atoms and organic carbons, the Te^- (reduction for CH_4) equals Te^- (oxidation for CO_2). The electron transfer (Te^-) among organic carbons drives the disproportionation of organic carbons to CH_4 and CO_2. The first part of organic carbons acts as electron-acceptor (gain of electrons) in the formation of CH_4 and the second part of organic carbons acts as electron-donor (loss of electrons) in the formation of CO_2. When the ON_C of an organic molecule is assigned, the corresponding value of $\frac{nCH_4}{nCO_2}$ can be determined. The ON_C on  equals +1, its ratio of nCH_4 to nCO_2 ($\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$) equals $\frac{3}{5}$.

5. Balancing Buswell's Equation and Counting Electron Transfer in $C_2H_5O_2N$'s Isomers

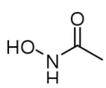
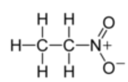
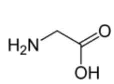
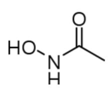
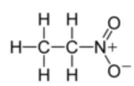
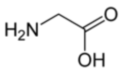
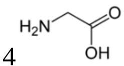
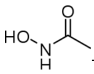
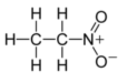
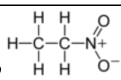
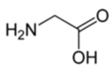
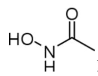
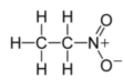
Using the procedures in Example 1 to work on isomers  and , their ON_N, ON_C, nH_2O, nCH_4, nCO_2, and Te^- are calculated. The three isomers of $C_2H_5O_2N$, , , and , correspond to their designated N-products of NH_3 ($ON_N = -3$), NH_2OH ($ON_N = -1$), and HNO_2 ($ON_N = +3$) respectively. Their ON_N, ON_C, SC, and Te^- are summarized in Table 1.

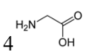
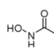
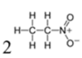
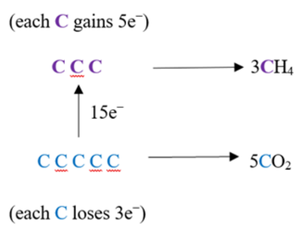
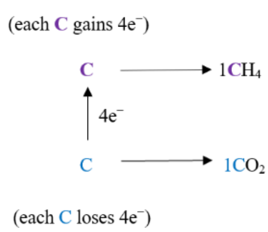
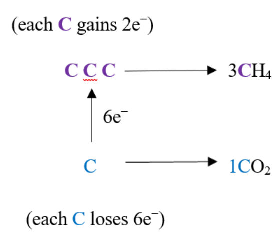
Table 1. BEq's parameters in three $C_2H_5O_2N$ isomers

Equation #	Balanced Buswell's equation	ON_N	ON_C	nH_2O	nCH_4	nCO_2	Te^-
1	 $+\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$	−3	+1	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{5}{4}$	$\frac{15}{4}$
2	4  $+2H_2O \rightarrow 3CH_4+5CO_2+4NH_3$	−3	+1	2	3	5	15
3	 $+H_2O \rightarrow CH_4+CO_2+NH_2OH$	−1	0	1	1	1	4
4	 $+H_2O \rightarrow \frac{3}{2}CH_4+\frac{1}{2}CO_2+HNO_2$	+3	−2	1	$\frac{3}{2}$	$\frac{1}{2}$	3
5	2  $+2H_2O \rightarrow 3CH_4+CO_2+2HNO_2$	+3	−2	2	3	1	6

Three different ON_C of $C_2H_5O_2N$ isomers have different Te^- among organic carbons in their own BEq. The 8 carbon atoms of 4  molecules disproportionate to 3 CH_4 molecules and 5 CO_2 molecules by exchanging 15 electrons from the group of 3 carbons to the other group of 5 carbons. The 1  molecule containing 2 carbon atoms disproportionate to 1 CH_4 molecule and 1 CO_2 molecule by exchanging 4 electrons. The 2  molecules (4 carbons) disproportionate to 3 CH_4 molecules and 1 CO_2 molecule by exchanging 6 electrons.

For the three $C_2H_5O_2N$ isomers, their Micro-BEq, ON_N, ON_C, Te^-, and BEq-Te^- diagrams are demonstrated in Table 2.

Table 2. BEq's parameters and BEq-Te^- diagrams for three $C_2H_5O_2N$ isomers

Micro-BEq	4  $+2H_2O \rightarrow 3CH_4+5CO_2+4NH_3$	 $+H_2O \rightarrow CH_4+CO_2+NH_2OH$	2  $+2H_2O \rightarrow 3CH_4+CO_2+2HNO_2$
ON_N	−3	−1	+3
ON_C	+1	0	−2
Disproportionation	8C → 3C + 5C	2C → C + C	4C → 3C + C
Te^-	15	4	6
BEq-Te^- diagram			

6. Deducing General Buswell's Equation of $C_xH_yO_zN_v$

Using the same strategy that was shown in Example 1, $C_xH_yO_zN_v$ is used for deducing the BEq equation.

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

Example 2. Balancing the BEq reaction of $C_xH_yO_zN_v$ ($ON_N = -3$) where NH_3 ($ON_N = -3$) is chosen as an N-product.

Step 1. Balance the BEq reaction: $C_xH_yO_zN_v+H_2O \rightarrow CH_4+CO_2+NH_3$

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

Step 2. Identify SC: nH_2O, nCH_4, and nCO_2

The BEq's SC of $nH_2O = \frac{4x-y-2z+3v}{4}$, $nCH_4 = \frac{4x+y-2z-3v}{8}$, and $nCO_2 = \frac{4x-y+2z+3v}{8}$ can be identified.

Step 3. Count Te^-

Reduction:	Oxidation:
$C_xH_yO_zN_v \rightarrow nCH_4\ CH_4$ $Te^- = nCH_4\ \Delta ON_{C1}$ $nCH_4 = \frac{4x+y-2z-3v}{8}$ $\Delta ON_C = ON_C(CH_4) - ON_C(C_xH_yO_zN_v)$ $\Delta ON_C = (-4) - ON_C(C_xH_yO_zN_v)$ $Te^- = nCH_4\ \Delta ON_{C1}$ $= nCH_4 [(-4) - ON_C(C_xH_yO_zN_v)]$ $\because nCH_4 = \frac{4x+y-2z-3v}{8}$; $ON_C(C_xH_yO_zN_v) = \frac{-y+2z+3v}{x}$ $\therefore Te^- = \frac{4x+y-2z-3v}{8}[(-4) - (\frac{-y+2z+3v}{x})]$ $= -\frac{(4x-y+2z+3v)(4x+y-2z-3v)}{8x}$	$C_xH_yO_zN_v \rightarrow nCO_2\ CO_2$ $Te^- = nCO_2\ \Delta ON_{C2}$ $nCO_2 = \frac{4x-y+2z+3v}{8}$ $\Delta ON_C = ON_C(CO_2) - ON_C(C_xH_yO_zN_v)$ $\Delta ON_C = (+4) - ON_C(C_xH_yO_zN_v)$ $Te^- = nCO_2\ \Delta ON_{C2}$ $= nCO_2 [(+4) - ON_C(C_xH_yO_zN_v)]$ $\because nCO_2 = \frac{4x-y+2z+3v}{8}$; $ON_C(C_xH_yO_zN_v) = \frac{-y+2z+3v}{x}$ $\therefore Te^- = \frac{4x-y+2z+3v}{8}[(+4) - (\frac{-y+2z+3v}{x})]$ $= +\frac{(4x-y+2z+3v)(4x+y-2z-3v)}{8x}$

Using the same procedures shown in Example 2, different N-products are assigned by their corresponding ON_N. The values of their ON_N, ON_C, nCH_4, nCO_2, and Te^- are given in Table 3.

Table 3. Stoichiometric coefficients and parameters (ON_N, ON_C, nCH_4 and nCO_2, and Te^-) in the balanced BEq of $C_xH_yO_zN_v$

Unbalanced Buswell's equation	ON_N	ON_C	nCH_4	nCO_2	Te^-
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + NH_3$	−3	$\frac{-y+2z+3v}{x}$	$\frac{4x+y-2z-3v}{8}$	$\frac{4x-y+2z+3v}{8}$	$\frac{(4x+y-2z-3v)(4x-y+2z+3v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + N_2H_4$	−2	$\frac{-y+2z+2v}{x}$	$\frac{4x+y-2z-2v}{8}$	$\frac{4x-y+2z+2v}{8}$	$\frac{(4x+y-2z-2v)(4x-y+2z+2v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + NH_2OH$	−1	$\frac{-y+2z+v}{x}$	$\frac{4x+y-2z-v}{8}$	$\frac{4x-y+2z+v}{8}$	$\frac{(4x+y-2z-v)(4x-y+2z+v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + N_2$	0	$\frac{-y+2z}{x}$	$\frac{4x+y-2z}{8}$	$\frac{4x-y+2z}{8}$	$\frac{(4x+y-2z)(4x-y+2z)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + N_2O$	+1	$\frac{-y+2z-v}{x}$	$\frac{4x+y-2z+v}{8}$	$\frac{4x-y+2z-v}{8}$	$\frac{(4x+y-2z+v)(4x-y+2z-v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + NO$	+2	$\frac{-y+2z-2v}{x}$	$\frac{4x+y-2z+2v}{8}$	$\frac{4x-y+2z-2v}{8}$	$\frac{(4x+y-2z+2v)(4x-y+2z-2v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + HNO_2$	+3	$\frac{-y+2z-3v}{x}$	$\frac{4x+y-2z+3v}{8}$	$\frac{4x-y+2z-3v}{8}$	$\frac{(4x+y-2z+3v)(4x-y+2z-3v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + NO_2$	+4	$\frac{-y+2z-4v}{x}$	$\frac{4x+y-2z+4v}{8}$	$\frac{4x-y+2z-4v}{8}$	$\frac{(4x+y-2z+4v)(4x-y+2z-4v)}{8x}$
$C_xH_yO_zN_v + H_2O \rightarrow CH_4 + CO_2 + HNO_3$	+5	$\frac{-y+2z-5v}{x}$	$\frac{4x+y-2z+5v}{8}$	$\frac{4x-y+2z-5v}{8}$	$\frac{(4x+y-2z+5v)(4x-y+2z-5v)}{8x}$

The ON_N in molecule $C_xH_yO_zN_v$ matches the ON_N in the designated product. For example, when the [N-product] is HNO_2 ($ON_N = +3$), the ON_N in molecule $C_xH_yO_zN_v$ must equal to +3. With reference to Table 3, the relationships between AC, ON_N, ON_C, SC, and Te^- in BEq are established. With any given structural formula of $C_xH_yO_zN_v$, the ON_C, nCH_4, nCO_2, and Te^- can be determined by the derived mathematical equations.

In summary, when $ON_H = +1$, $ON_O = -2$, and $\Sigma ON_{inc} = (y - 2z + ON_N\ v)$

$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(y-2z+ON_N\ v)}{x}$$

$$x\ ON_C = -(y - 2z + ON_N\ v)$$

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

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

$$Te^-\ (\text{oxidation}) = +\frac{(4x+y-2z+ON_N\ v)(4x-y+2z-ON_N\ v)}{8x} = +\frac{x(4-ONc)(4+ONc)}{8}$$

The "+" sign represents there is a loss of electrons.

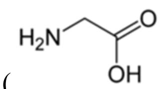
$$Te^-\ (\text{reduction}) = -\frac{(4x+y-2z+ON_N\ v)(4x-y+2z-ON_N\ v)}{8x} = -\frac{x(4-ONc)(4+ONc)}{8}$$

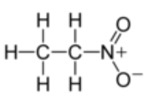
The "−" sign represents there is a gain of electrons.

$$Te^- = \frac{(4x+y-2z+ON_N\ v)(4x-y+2z-ON_N\ v)}{8x} = \frac{x(4-ONc)(4+ONc)}{8}$$

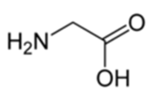
When there is neither a "+" nor "–", Te^- represents the number of transferred electrons among organic carbons in overall BEqs.

7. From Counting Te^- to Balancing Buswell's Equation for $C_xH_yO_zN_v$ Molecules

The operating procedures for counting Te^- and balancing BEq are provided. In Examples 3, 4, and 5 (with reference to Eq1 and Eq2), the same empirical formula ($C_2H_5O_2N$) shows two different structural formulas (

and 

).

Example 3. Given 

($C_2H_5O_2N$)

(a) Assign ON_{inc} and ON_C

Atom	C	H	O	N
ON_{inc}	-	+1	−2	−3
AC	2	5	2	1

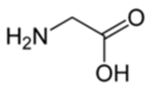
$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(ON_H\ y+ON_O\ z+ON_N\ v)}{x}$$

$$= \frac{-[(+1)(5)+(-2)(2)+(-3)(1)]}{2} = +1$$

(b) Determine nCH_4, nCO_2, and Te^-

x	ON_C	$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = x - nCH_4$	$Te^- = \frac{x(4-ONc)(4+ONc)}{8}$
2	+1	$nCH_4 = \frac{2[(4)-(+1)]}{8} = \frac{3}{4}$	$nCO_2 = 2 - \frac{3}{4} = \frac{5}{4}$	$Te^- = \frac{2[(4-(+1)][(4+(1)]}{8} = \frac{15}{4}$

(c) Balance Macro-BEq

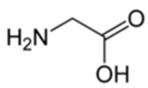


$+ \text{ nH}_2\text{O } H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$

Balance O atom:

$$2 + nH_2O = \frac{5}{2}$$

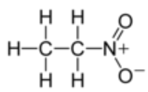
$$nH_2O = \frac{1}{2}$$



$+ \frac{1}{2}\ H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3,\ Te^- = \frac{15}{4}$

(d) Interpret Te^-

Since $\Delta ON_H = 0$, $\Delta ON_O = 0$, and $\Delta ON_N = 0$, there is no electron transfer among carbon atoms and non-carbon atoms. The Te^- among organic carbons, therefore, equals $\frac{15}{4}$.

Example 4. Given  ($C_2H_5O_2N$)

(a) Assign ON_{inc} and ON_C

Atom	C	H	O	N
ON_{inc}	-	+1	−1	+3
AC	2	5	2	1

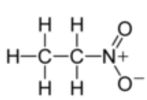
$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(ON_H\ y + ON_O\ z + ON_N\ v)}{x}$$

$$= \frac{-[(+1)(5)+(-1)(2)+(+3)\ (1)]}{3} = -2$$

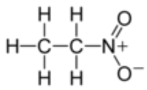
(b) Determine nCH_4, nCO_2, and Te^-

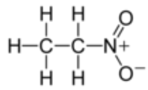
x	ON_C	$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = x - nCH_4$	$Te^- = \frac{x(4-ONc)(4+ONc)}{8}$
2	−2	$nCH_4 = \frac{2[(4)-(-2)]}{8} = \frac{3}{2}$	$nCO_2 = 2 - \frac{3}{2} = \frac{1}{2}$	$Te^- = \frac{2[(4-(-2)][(4+(-2)]}{8} = 3$

(c) Balance Macro-BEq

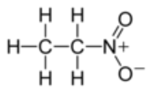


$+ \text{nH}_2\text{O } H_2O \rightarrow \frac{3}{2}CH_4 + \frac{1}{2}CO_2 + \text{[N-product]}$

Identify  ($ON_N = +3$):

When ON_N of nitrogen atom in  equals +3, the [N-product] is chosen as HNO_2 (ON_N= +3).

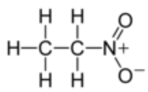
Balance N atom:

 $+nH_2O\ H_2O \rightarrow \frac{3}{2}CH_4 + \frac{1}{2}CO_2 + HNO_2$

Balance O atom for counting nH_2O:

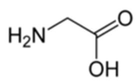
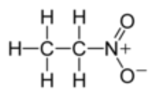
$2 + nH_2O = 1 + 2$

$nH_2O = 1$

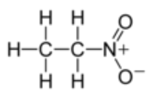
 $+H_2O \rightarrow \frac{3}{2}CH_4 + \frac{1}{2}CO_2 + HNO_2$, $Te^- = 3$

(d) Interpret Te^-

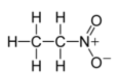
Since Te^- (reduction for CH_4) = Te^- (oxidation for CO_2), the Te^- among organic carbons equals 3.

In Examples 3 and 4, the ON_C of  and  cause different Te^- and $\frac{nCH_4}{nCO_2}$ in BEq. In other words, they are two different BEqs.

In Example 5, identify whether the given stoichiometric chemical equation is a BEq.

Example 5. Given  $(C_2H_5O_2N) + \frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4 + \frac{5}{4}CO_2 + NH_3$

(a) Assign ON_{inc}

Reactants		Products		
	H_2O	CH_4	CO_2	NH_3
$ON_H = +1$, $ON_O = -2$, $ON_N = +3$	$ON_H = +1$, $ON_O = -2$	$ON_H = +1$	$ON_O = -2$	$ON_N = -3$

(b) Compare ON_{inc} before and after the reaction

Before the reaction	After the reaction	Change in ON_{inc}
$ON_H = +1$	$ON_H = +1$	$\Delta ON_H = 0$
$ON_O = -2$	$ON_O = -2$	$\Delta ON_O = 0$
$ON_N = +3$	$ON_N = -3$	$\Delta ON_N \neq 0$

(c) Identify whether it is a BEq using Te^-

$\Sigma Te^- = Te^-(C1\ for\ CH_4) + Te^-(C2\ for\ CO_2) + Te^-(H) + Te^-(O) + Te^-(N)$

$0 = nCH_4\ \Delta ON_{C1} + nCO_2\ \Delta ON_{C2} + n_H\ \Delta ON_H + n_O\ \Delta ON_O + n_N\ \Delta ON_N$

$\because \Delta ON_{C1} \neq 0, \Delta ON_{C2} \neq 0, \Delta ON_H = 0, \Delta ON_O = 0, \Delta ON_N \neq 0$

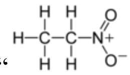
$\therefore 0 = nCH_4\ \Delta ON_{C1} + nCO_2\ \Delta ON_{C2} + n_N\ \Delta ON_N$

Since $\Delta ON_N = [(-3)-(+3)] = -6 < 0$, the N atom ($ON_N = +3$) gains electrons from organic carbons.

$\because$ 0 = $nCH_4\ \Delta ON_{C1}$ (gain of electrons) + $nCO_2\ \Delta ON_{C2}$ (loss of electrons) + $n_N\ \Delta ON_N$ (gain of electrons)

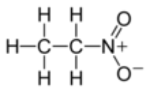
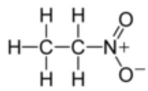
$\therefore$ Te^- (reduction for CH_4) ≠ Te^- (oxidation for CO_2)

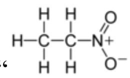
Since there is electron transfer from carbon atoms (loss of electrons) to nitrogen atom ($\Delta ON_N < 0$; gain of electrons), Te^- (reduction for CH_4) is not equal to Te^- (oxidation for CO_2). Therefore, the given stoichiometric chemical equation

"  ($C_2H_5O_2N$)+$\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$" is not a BEq.

(d) Identify whether it is a BEq using BEq-Ratio

BEq-Ratio: $\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$

Structural formula (SF)	Balanced chemical equation (Eq)
	 ($C_2H_5O_2N$)+$\frac{1}{2}H_2O \rightarrow \frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$
$ON_C = -2$ $\frac{(4-ONc)}{(4+ONc)} = \frac{[4-(-2)]}{[4+(-2)]} = 3$	$nCH_4 = \frac{3}{4}$, $nCO_2 = \frac{5}{4}$ $\frac{nCH_4}{nCO_2} = \frac{3}{5}$

Since the SF's $\frac{(4-ONc)}{(4+ONc)}$ (= 3) is not equal to the Eq's $\frac{nCH_4}{nCO_2}$ (= $\frac{3}{5}$), the Eq of "  ($C_2H_5O_2N$) +$\frac{1}{2}H_2O \rightarrow$

$\frac{3}{4}CH_4+\frac{5}{4}CO_2+NH_3$" is not a BEq.

8. Deriving Mathematical Relationships in General Buswell's Equation of $C_xH_yO_zX_wN_vS_uP_t$

The strategy above, which is used for balancing and deducing $C_xH_yO_zN_v$, can be extended to work on organic molecules containing the formula $C_xH_yO_zX_wN_vS_uP_t$. All possible ON_{inc} are: ON_H = +1 or −1, ON_O = −1 or −2, ON_X = integers between −1 and +7, ON_N = integers between −3 and +5, ON_S = integers between −2 and +6, and ON_P = integers between −3 and +5. The unbalanced general BEq equation is shown as:

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

All ON_{inc} in $C_xH_yO_zX_wN_vS_uP_t$ molecules remain the same before and after the reactions, therefore, $\Delta ON_H = 0$, $\Delta ON_O = 0$, $\Delta ON_X = 0$, $\Delta ON_N = 0$, $\Delta ON_S = 0$, and $\Delta ON_P = 0$.

With reference to Example 2, all ON_{inc}, ON_C, SC, and Te^- of $C_xH_yO_zX_wN_vS_uP_t$ in BEq can be determined.

In summary: $ONc = \frac{-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)}{x}$

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

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

$$Te^- = \frac{[4x+(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)][4x-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,)]}{8x}$$

8.1 Relationships between ON_C, ON_{inc}, nCH_4, and nCO_2

For $C_xH_yO_zX_wN_vS_uP_t$ molecules:

$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)}{x}$$

$$ON_C\,x = -\Sigma ON_{inc} = -(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)$$

where nc = x = number of organic carbons

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

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

8.2 Relationships between Te^-, AC, and ΣON_{inc}

$$\Sigma ON_{inc} = -(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)$$

$$Te^- = \frac{[4x+(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)][4x-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)]}{8x}$$

$$Te^- = \frac{(4x-\Sigma ON_{inc})(4x+\Sigma ON_{inc})}{8x}$$

8.3 Relationships between Te^-, ON_C, and AC

$$ON_C\,x = -(ON_H\,y+ON_O\,z+ON_N\,v+ON_S\,u+ON_P\,t)$$

$$Te^- = \frac{[4x+(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)][4x-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)]}{8x}$$

$$Te^- = \frac{x(4-ONc)(4+ONc)}{8}$$

8.4 Relationships between Te^-, ON_C, x, nCH_4, and nCO_2

$$Te^- = \frac{x(4-ONc)(4+ONc)}{8}$$

$$x = nCH_4 + nCO_2$$

$$nCO_2 = x - nCH_4$$

$$nCH_4 = \frac{x(4-ONc)}{8}$$

$$nCO_2 = \frac{x(4+ONc)}{8}$$

$$Te^- = nCH_4\,(4+ON_C)$$

$$Te^- = nCO_2\,(4-ON_C)$$

$$Te^- = (x-nCH_4)(4-ON_C)$$

8.5 Relationships between Te^-, ON_{inc}, ON_C, AC, nCH_4, and nCO_2

Mathematical equations for counting Te^- of $C_xH_yO_zX_wN_vS_uP_t$ are summarized in Table 4. Relationships between AC, ON_{inc}, ON_C, nCH_4, nCO_2, and Te^- are shown in Figure 2.

Table 4. Mathematical equations for counting Te^{-} of $C_xH_yO_zX_wN_vS_uP_t$ in BEq

Parameters	Mathematical equations for counting Te^{-}
AC, ON_{inc}	$Te^{-} = \frac{[4x+(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t][4x-(ON_H\,y+ON_O\,z+ON_X\,w+ON_N\,v+ON_S\,u+ON_P\,t)]}{8x}$
AC, ΣON_{inc}	$Te^{-} = \frac{(4x-\Sigma ON_{inc})(4x+\Sigma ON_{inc})}{8x}$
ON_C, x	$Te^{-} = \frac{x(4-ONc)(4+ONc)}{8}$
nCH_4, ON_C	$Te^{-} = nCH_4\,(4+ON_C)$
nCO_2, ON_C	$Te^{-} = nCO_2\,(4-ON_C)$
nCH_4, ON_C, x	$Te^{-} = (x-nCH_4)(4-ON_C)$

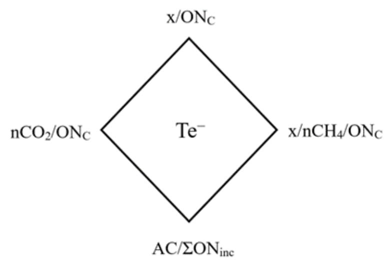


Figure 2. Relationships between AC, ON_{inc}, ON_C, nCH_4, nCO_2, and Te^{-}

8.6 Relationships between ON_C, Te^{-}, and nCH_4

Based on the mathematical equations of $nCH_4 = \frac{x(4-ONc)}{8}$ and $Te^{-} = \frac{x(4-ONc)(4+ONc)}{8}$, $Te^{-} = nCH_4\,(4+ON_C)$ is derived.

The triangular relationships between ON_C, nCH_4, and Te^{-} are shown in Figure 3.

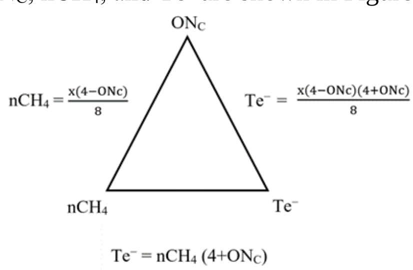


Figure 3 Triangular relationships between ON_C, nCH_4, and Te^{-}

8.7 Buswell-Electron and Buswell-Ratio

When electron transfer occurs only among organic carbons but not among non-carbon atoms and organic carbons, the Te^{-} drives the disproportionation of organic carbons to the formations of nCH_4 and nCO_2 in a fixed ratio. Figure 4 shows the relationships between ON_C, Buswell-Electron, and Buswell-Ratio.

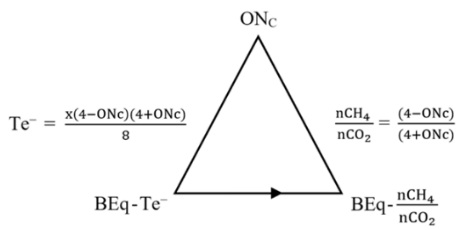
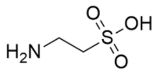


Figure 4. Relationships between ON_C, Buswell-Electron, and Buswell-Ratio

9. Operating Scheme for Counting Electron Transfer, Balancing Buswell's Equation, and Demonstrating BEq-Te⁻ Diagram

With any given structural formula of $C_xH_yO_zX_wN_vS_uP_t$, the nCH_4 and Te^- in BEq can be determined by the derived mathematical equations. The operating scheme is as follows:

Identify a structural formula → Assign ON_{inc}, ON_C → Determine nCH_4, nCO_2, Te^- → Balance Macro-BEq → Balance Micro-BEq → Draw BEq-Te^- diagram

Example 6. Given Taurine,  , $C_2H_7O_3NS$

(a) Assign ON_{inc} and ON_C

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

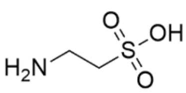
$$ON_C = \frac{-\Sigma ON_{inc}}{x} = \frac{-(ON_H\, y + ON_O\, z + ON_N\, v + ON_S\, u)}{x}$$

$$ON_C = \frac{-[(+1)7+(-2)\,(3)+(-3)(1)+(+4)(1)]}{2} = -1$$

(b) Determine nCH_4, nCO_2, and Te^-

x	ON_C	$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = x - nCH_4$	$Te^- = nCH_4\,(4+ON_C)$
2	−1	$nCH_4 = \frac{2[4-(-1)]}{8} = \frac{5}{4}$	$nCO_2 = 2 - \frac{5}{4} = \frac{3}{4}$	$Te^- = (\frac{5}{4})[4+(-1)] = \frac{15}{4}$

(c) Balance Macro-BEq

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

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

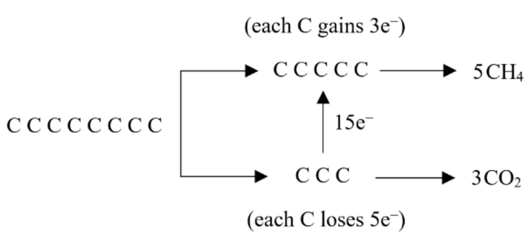
$nH_2O = \frac{1}{2}$

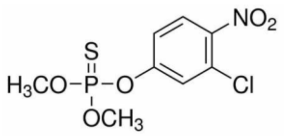
$C_2H_7O_3NS + \frac{1}{2}H_2O \rightarrow \frac{5}{4}CH_4 + \frac{3}{4}CO_2 + NH_3 + SO_2$, $Te^- = \frac{15}{4}$

(d) Balance Micro-BEq

$4C_2H_7O_3NS + 2H_2O \rightarrow 5CH_4 + 3CO_2 + 4NH_3 + 4SO_2$, $Te^- = 15$

(e) Draw BEq-Te^- diagram (disproportionation: 8C → 5C + 3C)



Example 7. Given Chlorthion,  , $C_8H_9O_5ClNSP$

(a) Assign ON_{inc} and ON_C

Atom	C	H	O	Cl	N	S	P
ON_{inc}	-	+1	−2	−1	+3	−2	+5
AC	8	9	5	1	1	1	1

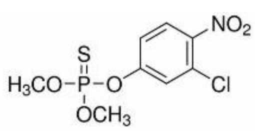
$$ON_C = \frac{-(ON_H\, y+ON_O\, z+ON_X\, w+ON_N\, v+ON_S\, u+ON_P\, t)}{x}$$

$$= \frac{-[(1)(9)+(-2)(5)+(-1)(1)+(+3)(1)+(-2)(1)+(+5)(1)]}{8} = -\frac{1}{2}$$

(b) Determine nCH_4, nCO_2, and Te^-

x	ON_C	$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = x - nCH_4$	$Te^- = nCH_4\,(4+ON_C)$
8	$-\frac{1}{2}$	$nCH_4 = \frac{8[(4)-(-\frac{1}{2})]}{8} = \frac{9}{2}$	$nCO_2 = 8 - \frac{9}{2} = \frac{7}{2}$	$Te^- = (\frac{9}{2})[4+(-\frac{1}{2})] = \frac{63}{4}$

(c) Balance Macro-BEq

 $(C_8H_9O_5ClNSP)+nH_2O\ H_2O \rightarrow \frac{9}{2}CH_4+\frac{7}{2}CO_2+HCl+HNO_2+H_2S+H_3PO_4$

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

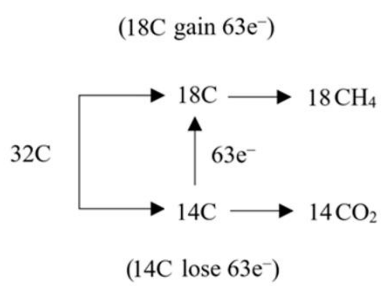
$nH_2O = 8$

$C_8H_9O_5ClNSP+8H_2O \rightarrow \frac{9}{2}CH_4+\frac{7}{2}CO_2+HCl+HNO_2+H_2S+H_3PO_4$, $Te^- = \frac{63}{4}$

(d) Balance Micro-BEq

$4C_8H_9O_5ClNSP+32H_2O \rightarrow 18CH_4+14CO_2+4HCl+4HNO_2+4H_2S+4H_3PO_4$, $Te^- = 63$

(e) Draw BEq-Te^- diagram (disproportionation: 32C → 18C + 14C)



10. Conclusions

Using ON_C as a redox metric for BEq, the relationships between ON_C, nCH_4, nCO_2, and Te^- are established. The number of transferred electrons on organic carbons drives the disproportionation to the formations of CH_4 to CO_2 in a fixed molar ratio. Organic carbons are redox atoms whereas non-carbon atoms are non-redox atoms. With any known organic structural formula, three tasks can be achieved: (1) determination of the Buswell-Ratio ($\frac{nCH_4}{nCO_2} = \frac{(4-ONc)}{(4+ONc)}$), (2) counting of Buswell-Electron using $Te^- = \frac{x(4-ONc)(4+ONc)}{8}$, $Te^- = nCH_4\ (4+ON_C)$, or $Te^- = nCO_2\ (4-ON_C)$, and (3) demonstration of electron transfer among organic carbons by drawing the BEq-Te^- diagram. Furthermore, Buswell-Electron and Buswell-Ratio are developed as criteria for identifying whether a balanced chemical equation is a Buswell' s equation.

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Authors contributions

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

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Competing interests

There are no conflicts to declare.

Informed consent

Obtained.

Ethics approval

The Publication Ethics Committee of the Canadian Center of Science and Education.

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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 are not publicly available due to privacy or ethical restrictions.

Data sharing statement

No additional data are available.

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