Counting and Demonstrating Electron Transfer in Buswell’s Equation

Pong Kau Yuen¹, Cheng Man Diana Lau¹

¹Macau Chemical Society, Macao, Macao

Correspondence: Pong Kau Yuen, Macau Chemical Society, Macao, Macao. E-mail: pongkauyuen@yahoo.com

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Abstract

Anaerobic digestion is a microorganism-mediated redox system which is chemically represented by Buswell’s equation. In the equation, 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 among 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) determine the Buswell-Ratio, (2) count Buswell-Electron, and (3) demonstrate electron transfer among organic carbons by drawing the Buswell-Electron diagram.

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 an 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). The Buswell’s equation (BEq) is established to represent it chemically (Buswell & Mueller, 1952; Boyle (1977). Based on the elemental composition of organic matter, the equation counts quantity of biogas and digestates. The general balanced BEq for C₅H₇O₂X₆N₅S₁P₁ (Yuen & Lau, 2023a) is shown in the following:

\[
\text{C}_5\text{H}_7\text{O}_2\text{X}_6\text{N}_5\text{S}_1\text{P}_1 + \frac{4x-y-2z+w+3v+2u+11t}{4} \text{H}_2\text{O} \rightarrow \frac{4x+y-2z-w-3v-2u+5t}{8} \text{CH}_4 + \frac{4x-y+2z+w+3v+2u-5t}{8} \text{CO}_2 + \text{vHX} + \text{wH}_2\text{S} + \text{tH}_3\text{PO}_4
\]

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 CH₄ and CO₂, and (iv) all heteroatoms (halogen, nitrogen, sulfur, and phosphorous) convert to HX, NH₃, H₂S, and H₃PO₄, respectively. The significance of quantity of methane \((n\text{CH}_4)\) 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 \((n\text{CH}_4)\) and carbon dioxide \((n\text{CO}_2)\). To illustrate this, two different stoichiometric chemical equations of \((\text{C}_2\text{H}_4\text{O}_2\text{N})\) and \((\text{C}_2\text{H}_6\text{O}_2\text{N})\) are shown in the following:

Eq1: \(\text{H}_2\text{N} \rightarrow \frac{1}{2} \text{H}_2\text{O} \rightarrow \frac{3}{4} \text{CH}_4 + \frac{5}{4} \text{CO}_2 + \text{NH}_3\)

Eq2: \(\text{H}_2\text{N} \rightarrow \frac{1}{2} \text{H}_2\text{O} \rightarrow \frac{3}{4} \text{CH}_4 + \frac{5}{4} \text{CO}_2 + \text{NH}_3\)
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, Virdis & Batstone, 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, Nevin & Lovley, 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, 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 (ONc) not only serves as a redox indicator of organic matter, also a valuable redox metric for understanding organic carbon’s characteristics. ONc 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 ONc and nCH4 in BEq has already been established (Yuen & Lau, 2024a), there is still a conceptual void among ONc, nCH4, and Te−. 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, ONc is a key redox parameter to explore the redox nature of BEq. The aims of this article are (i) to establish the relationships among ONc, nCH4, 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 Carbon (ONc)

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

For organic matters: CxHyOzXwNvSwPtvcharge

\[ C, H, O, X, N, S, P = \text{carbon, hydrogen, oxygen, halogen, nitrogen, sulfur, and phosphorus elements} \]
\[ x, y, z, w, v, u, t = \text{atomic coefficients for C, H, O, X, N, S, P} \]
\[ \text{charge} = \text{electrical charge of organic matter} \]
\[ nc = x = \text{number of organic carbons} \]
\[ \text{ON}_{inc} = \text{individual oxidation number of non-carbon atoms} \]
\[ AC = \text{atomic coefficients} \]

When charge ≠ 0, \( ONc = \frac{\text{charge} - \Sigma ON_{inc}}{nc} \).

When charge = 0, \( ONc = \frac{-\Sigma ON_{inc}}{nc} \).

Given a structural formula of CxHyOzXwNvSwPtv

\[ C_{x}H_{y}O_{z}X_{w}N_{v}S_{u}P_{t} \]

\[ \text{AC} = x, y, z, w, v, u, t \]

\[ \Sigma ON_{inc} = [(ON_{H} y) + (ON_{O} z) + (ON_{X} w) + (ON_{N} v) + (ON_{S} u) + (ON_{P} t)] \]
The mathematical equation for calculating ON$_c$ is established for neutral organic molecules in their structural formulas:

$$\text{ON}_c = \frac{-\sum \text{ON}_{\text{inc}}}{n_c}$$

$$\text{ON}_c = \frac{-[(\text{ON}_N y) + (\text{ON}_O z) + (\text{ON}_X w) + (\text{ON}_N v) + (\text{ON}_S u) + (\text{ON}_P t)]}{x}$$

2.2 Isomers of Organonitrogen Molecules

The organonitrogen molecules, C$_2$H$_4$O$_2$N$_6$ and C$_2$H$_4$O$_2$N are chosen to illustrate the counting of Te$^-$ in BEq. Three selected structural formulas of C$_2$H$_4$O$_2$N$_6$ isomers are:

![Structural formula of isomers](http://ijc.ccsenet.org)

An empirical formula shows its elemental composition only, and a structural formula identifies 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$_2$O are balancing tools. It can be used to balance, deduce, quantify, and define redox reactions (Yuen & Lau; 2022c). It can also be used to understand BEq (Yuen & Lau; 2024a).

2.4 Organic Redox Couples

In a balanced half organic redox reaction, the mathematical equation is Te$^-$ = nc $\Delta$ON$_c$ for organic redox couples (Yuen & Lau, 2022c; 2023a). Changes in mean oxidation number of organic carbons ($\Delta$ON$_c$) of two organic redox couples in BEq are shown in the following:

$$\Delta \text{ON}_c = \text{ON}_c (\text{CH}_4) - \text{ON}_c (\text{organic molecule})$$

$$\Delta \text{ON}_c = \text{ON}_c (\text{CO}_2) - \text{ON}_c (\text{organic molecule})$$

2.5 Buswell’s Equation (BEq)

When empirical formulas of organic matter are given, the general balanced BEq for C$_8$H$_{15}$O$_x$N$_y$S$_z$P$_t$ is shown in the following:

$$\text{C}_8\text{H}_{15}\text{O}_x\text{N}_y\text{S}_z\text{P}_t + \frac{4x-y-2z+w+3v+2u+11t}{4} \text{H}_2\text{O} \rightarrow \frac{4x+y-2z-w-3v-2u+5t}{8} \text{CH}_4 + \frac{4x-y+2z+w+3v+2u-5t}{8} \text{CO}_2 + w\text{HX} + v\text{NH}_3 + u\text{H}_2\text{S} + t\text{H}_3\text{PO}_4$$

Based on the elemental composition, the nCH$_4$, nCO$_2$, and $\frac{n\text{CH}_4}{n\text{CO}_2}$ can be determined by the following mathematical equations.

<table>
<thead>
<tr>
<th>$n\text{CH}_4$</th>
<th>$n\text{CO}_2$</th>
<th>$\frac{n\text{CH}_4}{n\text{CO}_2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{4x+y-2z-w-3v-2u+5t}{8}$</td>
<td>$\frac{4x-y+2z+w+3v+2u-5t}{8}$</td>
<td>$\frac{4x+y-2z-w-3v-2u+5t}{4x-y+2z+w+3v+2u-5t}$</td>
</tr>
</tbody>
</table>

2.6 ON$_c$-Buswell’s Equation (ON$_c$-BEq)

The general unbalanced BEq for C$_8$H$_{15}$O$_x$N$_y$S$_z$P$_t$ (Yuen & Lau; 2024a) is shown as:

$$\text{C}_8\text{H}_{15}\text{O}_x\text{N}_y\text{S}_z\text{P}_t + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{CO}_2 + [\text{H-product}] + [\text{O-product}] + [\text{X-product}] + [\text{N-product}] + [\text{S-product}] + [\text{P-product}]$$

Based on any structural formula of an organic molecule, the x, nCH$_4$, nCO$_2$, and $\frac{n\text{CH}_4}{n\text{CO}_2}$ can be determined by the following mathematical equations.

| x = nCH$_4$ + nCO$_2$ | nCH$_4$ = $\frac{x(4-\text{ON}_c)}{8}$ | nCO$_2$ = $\frac{x(4+\text{ON}_c)}{8}$ | $\frac{n\text{CH}_4}{n\text{CO}_2}$ = $\frac{4-x}{4+x}$ |

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

To count Te$^-$ in BEq, three procedures are needed: (i) use the structural formula method to assign ON, (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 $\rightarrow AC$, ON\textsubscript{inc}, and ON\textsubscript{C} $\rightarrow$ stoichiometric coefficients (SC) $\rightarrow$ Te$^-$.

Example 1. Given a structural formula

\[
\text{H}_2\text{N} \xrightarrow{\text{O}} \text{O} \xrightarrow{\text{H}} \text{OH}
\]

$(\text{C}_2\text{H}_5\text{O}_2\text{N})$, count the Te$^-$ in BEq

Step 1. Assign ON\textsubscript{inc} (ON\textsubscript{H}, ON\textsubscript{O}, and ON\textsubscript{N}) and ON\textsubscript{C}

Using fragmentation method,

1.1 Count ON\textsubscript{inc} of H$_2$N$^-$

ON\textsubscript{H} = +1, ON\textsubscript{N} = -3

1.2 Count ON\textsubscript{C} of OH

Using the non-carbon atom method, ON\textsubscript{C} can be counted by ON\textsubscript{inc} and AC.

\[
\begin{array}{cccc}
\text{Atom} & \text{C} & \text{H} & \text{O} & \text{N} \\
\text{ON}_{\text{inc}} & - & +1 & -2 & -3 \\
\text{AC} & 2 & 5 & 2 & 1
\end{array}
\]

\[
\text{ON}_{\text{C}} = \frac{-\sum \text{ON}_{\text{inc}}}{x} = \frac{-([+1]5+[-2]2+[-3]1)}{2} = +1
\]

The ON\textsubscript{C} on H$_2$N$^-$ equals +1.

Step 2. Balance BEq

2.1 Set up the unbalanced BEq

\[
\begin{align*}
\text{ON}_\text{N} \text{ of the reactant } (\quad) \text{ is identified as } -3. \\
\text{The NH}_3 \text{ (ON}_\text{N} = -3) \text{ is selected as the designated N-product accordingly.}
\end{align*}
\]

The unbalanced BEq is shown as:

\[
(\text{C}_2\text{H}_5\text{O}_2\text{N}) + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{CO}_2 + \text{NH}_3
\]

2.2 Balance BEq by using the H-atom method

Divide an overall equation into two half reactions

\[
\begin{align*}
\text{C}_2\text{H}_5\text{O}_2\text{N} & \rightarrow \text{CH}_4 + \text{NH}_3 \\
\text{C}_2\text{H}_5\text{O}_2\text{N} & \rightarrow \text{CO}_2 + \text{NH}_3
\end{align*}
\]

Balance two half reactions

\[
\begin{align*}
\text{C}_2\text{H}_5\text{O}_2\text{N} & \rightarrow \text{CH}_4 + \text{NH}_3 \\
\text{C}_2\text{H}_5\text{O}_2\text{N} + 10\text{H} & \rightarrow 2\text{CH}_4 + \text{NH}_3 + 2\text{H}_2\text{O} \\
\text{C}_2\text{H}_5\text{O}_2\text{N} & \rightarrow \text{CO}_2 + \text{NH}_3 \\
\text{C}_2\text{H}_5\text{O}_2\text{N} + 2\text{H}_2\text{O} & \rightarrow 2\text{CO}_2 + \text{NH}_3 + 6\text{H}
\end{align*}
\]

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

\[
(\text{C}_2\text{H}_5\text{O}_2\text{N} + 10\text{H} \rightarrow 2\text{CH}_4 + \text{NH}_3 + 2\text{H}_2\text{O}) \times 3
\]

\[
(\text{C}_2\text{H}_5\text{O}_2\text{N} + 2\text{H}_2\text{O} \rightarrow 2\text{CO}_2 + \text{NH}_3 + 6\text{H}) \times 5
\]
\[
\begin{align*}
  &8 \text{H}_2\text{N}\text{CO} \rightarrow +4\text{H}_2\text{O} \rightarrow 6\text{CH}_4 + 10\text{CO}_2 + 8\text{NH}_3 \\
  &\text{OH} \rightarrow \text{H}_2\text{O} + \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3
\end{align*}
\]

The SC of \( n\text{H}_2\text{O} = \frac{1}{2} \), \( n\text{CH}_4 = \frac{3}{4} \), and \( n\text{CO}_2 = \frac{5}{4} \) can be identified by the balanced BEq.

Step 3. Count \( \text{Te}^- \)

Using the equation of \( \text{Te}^- = nc \Delta \text{ON}_C \) for organic redox couples, \( \text{Te}^- \) can be counted by the parameters \( \Delta \text{ON}_C, n\text{CH}_4, \) and \( n\text{CO}_2 \).

Based on the balanced BEq:

\[
+\frac{1}{2}\text{H}_2\text{O} \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3, \; \text{Te}^- = \frac{15}{4}
\]

the \( \text{Te}^- \) (reduction) and \( \text{Te}^- \) (oxidation) on carbon atoms can be determined as follows:

<table>
<thead>
<tr>
<th>Reduction: ( \text{Te}^- ) (reduction)</th>
<th>Oxidation: ( \text{Te}^- ) (oxidation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Te}^- = n\text{CH}_4 \Delta \text{ON}_C )</td>
<td>( \text{Te}^- = n\text{CO}_2 \Delta \text{ON}_C )</td>
</tr>
<tr>
<td>( = n\text{CH}_4 [\text{ON}_C (\text{CH}_4) - \text{ON}_C (\text{H}_2\text{O})] )</td>
<td>( = n\text{CO}_2 [\text{ON}_C (\text{CO}_2) - \text{ON}_C (\text{H}_2\text{O})] )</td>
</tr>
<tr>
<td>( = n\text{CH}_4 [(-4) - \text{ON}_C (\text{C}_2\text{H}_5\text{O}_2\text{N})] )</td>
<td>( = n\text{CO}_2 [(+4) - \text{ON}_C (\text{C}_2\text{H}_5\text{O}_2\text{N})] )</td>
</tr>
<tr>
<td>( \therefore n\text{CH}_4 = \frac{3}{4}; \text{ON}_C (\text{C}_2\text{H}_5\text{O}_2\text{N}) = +1 )</td>
<td>( \therefore n\text{CO}_2 = \frac{5}{4}; \text{ON}_C (\text{C}_2\text{H}_5\text{O}_2\text{N}) = +1 )</td>
</tr>
<tr>
<td>( \therefore \text{Te}^- = \frac{3}{4} [(-4) - (+1)] )</td>
<td>( \therefore \text{Te}^- = \frac{5}{4} [(+4) - (+1)] )</td>
</tr>
<tr>
<td>( = -\frac{15}{4} ) (a gain of ( \frac{15}{4} ) electrons)</td>
<td>( = +\frac{15}{4} ) (a loss of ( \frac{15}{4} ) electrons)</td>
</tr>
</tbody>
</table>

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:

\[
\text{H}_2\text{N}\text{CO} \rightarrow +\frac{1}{2}\text{H}_2\text{O} \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3, \; \text{Te}^- = \frac{15}{4}
\]

Macroscopically, 1 mole of \( \text{H}_2\text{N}\text{CO} \) involves \( \frac{15}{4} \) electrons disproportionate to \( \frac{3}{4} \) mole of \( \text{CH}_4 \) and \( \frac{5}{4} \) mole of \( \text{CO}_2 \).

\[
\begin{align*}
  \text{H}_2\text{N}\text{CO} \rightarrow +\frac{1}{2}\text{H}_2\text{O} & \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3, \; \text{Te}^- = \frac{15}{4} \\
  \frac{3}{4} \text{ mole of CH}_4 & \rightarrow (\text{Te}^- = \frac{15}{4})
\end{align*}
\]
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

\[
\text{H}_2\text{N}\text{COOH} + 2\text{H}_2\text{O} \rightarrow 3\text{CH}_4 + 5\text{CO}_2 + 4\text{NH}_3, \quad \text{Te}^- = 15.
\]

Microscopically, 4 molecules of involve 15 electrons disproportionate to 3 molecules of CH\(_4\) and 5 molecules of CO\(_2\).

\[
\begin{align*}
4 \text{ molecules} & \rightarrow 3 \text{ molecules of CH}_4 \\
& \rightarrow 5 \text{ molecules of CO}_2
\end{align*}
\]

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 molecules is shown in Figure 1.

\[
\begin{align*}
\text{H}_2\text{N}\text{COOH} & \rightarrow 3\text{CH}_4 \\
& \rightarrow 5\text{CO}_2
\end{align*}
\]

\[
\begin{align*}
\text{C C C C C C C C} & \rightarrow 3 \text{CH}_4 \\
& \rightarrow 5 \text{CO}_2
\end{align*}
\]

Figure 1. The BEq-Te\(^-\) diagram for molecules

4.4 Interpretation of Te\(^-\)

\[
\Sigma \text{Te}^- = \text{net number of transferred electrons in overall redox reactions}
\]

\[
\Sigma \text{Te}^- = 0
\]

For \(\text{C}_x\text{H}_y\text{O}_z\text{N}_v\) molecules,

\[
\Sigma \text{Te}^- = \text{Te}^- (\text{C}1 \text{ for CH}_4) + \text{Te}^- (\text{C}2 \text{ for CO}_2) + \text{Te}^- (\text{H}) + \text{Te}^- (\text{O}) + \text{Te}^- (\text{N})
\]

\[
\Sigma \text{Te}^- = n\text{CH}_4 \Delta \text{ON}_C + n\text{CO}_2 \Delta \text{ON}_C + n\text{H} \Delta \text{ON}_H + n\text{O} \Delta \text{ON}_O + n\text{N} \Delta \text{ON}_N
\]

When all ON\(_{inc}\) remain the same before and after a redox reaction, \(\Delta \text{ON}_H = 0, \Delta \text{ON}_O = 0,\) and \(\Delta \text{ON}_N = 0\) are attained. All non-carbon atoms are identified as non-redox atoms.

\[
0 = \text{Te}^- (\text{C}1 \text{ for CH}_4) + \text{Te}^- (\text{C}2 \text{ for CO}_2)
\]

\[
0 = n\text{CH}_4 \Delta \text{ON}_C1 \text{ (gain of electrons)} + n\text{CO}_2 \Delta \text{ON}_C2 \text{ (loss of electrons)}
\]

\[-n\text{CH}_4 \Delta \text{ON}_C1 = n\text{CO}_2 \Delta \text{ON}_C2\]
\[-n\text{CH}_4(-4\text{ONc}) = n\text{CO}_2(4\text{ONc})\]
\[n\text{CH}_4(4+\text{ONc}) = n\text{CO}_2(4-\text{ONc})\]
\[\frac{n\text{CH}_4}{n\text{CO}_2} = \frac{(4-\text{ONc})}{(4+\text{ONc})}\]

Te\(^-(\text{C1 for CH}_4\text{)}\) means Te\(^-\) (reduction for CH\(_4\))

Te\(^-(\text{C2 for CO}_2\text{)}\) means Te\(^-\) (oxidation for CO\(_2\))

When Te\(^-\) (reduction for CH\(_4\)) = Te\(^-\) (oxidation for CO\(_2\)), the mathematical relation of

\[\frac{n\text{CH}_4}{n\text{CO}_2} = \frac{(4-\text{ONc})}{(4+\text{ONc})}\]

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 \(\frac{n\text{CH}_4}{n\text{CO}_2}\) can be determined. The ON\(_C\) equals +1, its ratio of nCH\(_4\) to nCO\(_2\)

\(\left(\frac{n\text{CH}_4}{n\text{CO}_2}\right) = \frac{(4-\text{ONc})}{(4+\text{ONc})}\)

equals \(\frac{3}{5}\).

### 5. Balancing Buswell’s Equation and Counting Electron Transfer in C\(_2\)H\(_5\)O\(_2\)N’s Isomers

Using the procedures in Example 1 to work on isomers and, their ON\(_N\), ON\(_C\), nH\(_2\)O, nCH\(_4\), nCO\(_2\), and Te\(^-\) are calculated. The three isomers of C\(_2\)H\(_5\)O\(_2\)N, and, correspond to their designated N-products of NH\(_3\) (ON\(_N\) = −3), NH\(_2\)OH (ON\(_N\) = −1), and HNO\(_2\) (ON\(_N\) = +3) respectively. Their ON\(_N\), ON\(_C\), SC, and Te\(^-\) are summarized in Table 1.

<table>
<thead>
<tr>
<th>Equation #</th>
<th>Balanced Buswell’s equation</th>
<th>ON(_N)</th>
<th>ON(_C)</th>
<th>nH(_2)O</th>
<th>nCH(_4)</th>
<th>nCO(_2)</th>
<th>Te(^-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(-\frac{1}{2}\text{H}_2\text{O} - \frac{3}{4}\text{CH}_4 + 5\text{CO}_2 + \text{NH}_3)</td>
<td>−3</td>
<td>+1</td>
<td>(\frac{1}{2})</td>
<td>(\frac{3}{4})</td>
<td>(\frac{5}{4})</td>
<td>(\frac{15}{4})</td>
</tr>
<tr>
<td>2</td>
<td>(2\text{H}_2\text{O} \rightarrow 3\text{CH}_4 + 5\text{CO}_2 + 4\text{NH}_3)</td>
<td>−3</td>
<td>+1</td>
<td>2</td>
<td>3</td>
<td>5</td>
<td>15</td>
</tr>
<tr>
<td>3</td>
<td>(\text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{CO}_2 + \text{NH}_2\text{OH})</td>
<td>−1</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>4</td>
</tr>
<tr>
<td>4</td>
<td>(\frac{1}{2}\text{H}_2\text{O} - \frac{3}{2}\text{CH}_4 + \frac{1}{2}\text{CO}_2 + \text{HNO}_2)</td>
<td>+3</td>
<td>−2</td>
<td>1</td>
<td>(\frac{3}{2})</td>
<td>(\frac{1}{2})</td>
<td>3</td>
</tr>
<tr>
<td>5</td>
<td>(2\text{H}_2\text{O} \rightarrow 3\text{CH}_4 + 2\text{CO}_2 + 2\text{HNO}_2)</td>
<td>+3</td>
<td>−2</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>6</td>
</tr>
</tbody>
</table>

Three different ON\(_C\) of C\(_2\)H\(_5\)O\(_2\)N isomers have different Te\(^-\) among organic carbons in their own BEq. The 8 carbon
atoms of 4 molecules disproportionate to 3 CH4 molecules and 5 CO2 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 CH4 molecule and 1 CO2 molecule by exchanging 4 electrons. The 2 molecules (4 carbons) disproportionate to 3 CH4 molecules and 1 CO2 molecule by exchanging 6 electrons.

For the three C2H6O2N isomers, their Micro-BEq, ONN, ONC, Te–, and BEq–Te– diagrams are demonstrated in Table 2.

<table>
<thead>
<tr>
<th>Micro-BEq</th>
<th>ONN</th>
<th>ONC</th>
<th>Te–</th>
<th>Disproportionation</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>−3</td>
<td>+1</td>
<td>15</td>
<td>8C → 3C + 5C</td>
</tr>
<tr>
<td>2</td>
<td>−1</td>
<td>0</td>
<td>4</td>
<td>2C → C + C</td>
</tr>
<tr>
<td></td>
<td>+3</td>
<td>−2</td>
<td>6</td>
<td>4C → 3C + C</td>
</tr>
</tbody>
</table>

6. Deducing General Buswell’s Equation of C2H6O2N

Using the same strategy that was shown in Example 1, C2H6O2Nv is used for deducing the BEq equation. C2H6O2Nv + H2O → CH4 + CO2 + [N-product]

Example 2. Balancing the BEq reaction of C2H6O2Nv (ONN = −3) where NH3 (ONN = −3) is chosen as an N-product.

Step 1. Balance the BEq reaction: C2H6O2Nv + H2O → CH4 + CO2 + NH3

\[
\begin{align*}
\text{C}_2\text{H}_6\text{O}_2\text{N}_v + \text{H}_2\text{O} & \rightarrow 4x + 8y - 22 - 3v \\
\text{CH}_4 & \rightarrow 4x + 4y - 2x - 3v \\
\text{CO}_2 & \rightarrow 4x + y + 22 + 3v \\
\text{NH}_3 & \text{ is chosen as an } N\text{-product.}
\end{align*}
\]

Step 2. Identify SC: nH2O, nCH4, and nCO2

The BEq’s SC of nH2O = \(\frac{4x - y - 22 + 3y}{8}\), nCH4 = \(\frac{4x + y + 22 - 3v}{8}\), and nCO2 = \(\frac{4x - y + 22 + 3v}{8}\) can be identified.
Step 3. Count Te⁻

<table>
<thead>
<tr>
<th>Reduction:</th>
<th>Oxidation:</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₆H₁₀N₂₅ → nCH₄ CH₆</td>
<td>C₅H₅N₄ → nCO₂ CO₂</td>
</tr>
<tr>
<td>Te⁻ = nCH₄ ΔONc</td>
<td>Te⁻ = nCO₂ ΔONc</td>
</tr>
<tr>
<td>nCH₄ = \frac{4x+y−2z−3v}{8}</td>
<td>nCO₂ = \frac{4x−y+2z+3v}{8}</td>
</tr>
<tr>
<td>ΔONc = ONc (CH₄) − ONc (C₅H₅N₄)</td>
<td>ΔONc = ONc (CO₂) − ONc (C₅H₅N₄)</td>
</tr>
<tr>
<td>ΔONc = (−4) − ONc (C₅H₅N₄)</td>
<td>ΔONc = (+4) − ONc (C₅H₅N₄)</td>
</tr>
<tr>
<td>Te⁻ = nCH₄ ΔONc</td>
<td>Te⁻ = nCO₂ ΔONc</td>
</tr>
<tr>
<td>= nCH₄ [(−4) − ONc (C₅H₅N₄)]</td>
<td>= nCO₂ [(+4) − ONc (C₅H₅N₄)]</td>
</tr>
<tr>
<td>\therefore nCH₄ = \frac{4x+y−2z−3v}{8}; ONc (C₅H₅N₄) = \frac{−y+2z+3v}{x}</td>
<td>\therefore nCO₂ = \frac{4x−y+2z+3v}{8}; ONc (C₅H₅N₄) = \frac{−y+2z+3v}{x}</td>
</tr>
<tr>
<td>\therefore Te⁻ = \frac{4x+y−2z−3v}{8} \left[(−4) − \left(\frac{−y+2z+3v}{x}\right)\right]</td>
<td>\therefore Te⁻ = \frac{4x−y+2z+3v}{8} \left[(+4) − \left(\frac{−y+2z+3v}{x}\right)\right]</td>
</tr>
<tr>
<td>= \left(\frac{4x−y+2z+3v\cdot(4x+y−2z−3v)}{8x}\right)</td>
<td>= \left(\frac{4x−y+2z+3v\cdot(4x+y−2z−3v)}{8x}\right)</td>
</tr>
</tbody>
</table>

Using the same procedures shown in Example 2, different N-products are assigned by their corresponding ONₙ. The values of their ONₙ, ONc, nCH₄, nCO₂, and Te⁻ are given in Table 3.

Table 3. Stoichiometric coefficients and parameters (ONₙ, ONc, nCH₄ and nCO₂, and Te⁻) in the balanced BEq of C₅H₅N₄.

<table>
<thead>
<tr>
<th>Unbalanced Buswell’s equation</th>
<th>ONₙ</th>
<th>ONc</th>
<th>nCH₄</th>
<th>nCO₂</th>
<th>Te⁻</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + NH₃</td>
<td>−3</td>
<td>\frac{−y + 2z + 3v}{x}</td>
<td>\frac{4x − y − 2z − 3v}{8}</td>
<td>\frac{4x − y + 2z + 3v}{8}</td>
<td>(\frac{4x + y − 2z − 3v\cdot(4x − y + 2z + 3v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + N₂H₄</td>
<td>−2</td>
<td>\frac{−y + 2z + 2v}{x}</td>
<td>\frac{4x + y − 2z − 2v}{8}</td>
<td>\frac{4x − y + 2z + 2v}{8}</td>
<td>(\frac{4x + y + 2z − 2v\cdot(4x − y + 2z + 2v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + NH₂OH</td>
<td>−1</td>
<td>\frac{−y + 2z + v}{x}</td>
<td>\frac{4x + y − 2z − v}{8}</td>
<td>\frac{4x − y + 2z + v}{8}</td>
<td>(\frac{4x + y − 2z − v\cdot(4x − y + 2z + v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + N₂</td>
<td>0</td>
<td>\frac{−y + 2z}{x}</td>
<td>\frac{4x + y − 2z}{8}</td>
<td>\frac{4x − y + 2z}{8}</td>
<td>(\frac{4x + y − 2z\cdot(4x − y + 2z)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + NO</td>
<td>+1</td>
<td>\frac{−y + 2z − v}{x}</td>
<td>\frac{4x + y − 2z + v}{8}</td>
<td>\frac{4x − y + 2z − v}{8}</td>
<td>(\frac{4x + y − 2z + v\cdot(4x − y + 2z − v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + NO₂</td>
<td>+2</td>
<td>\frac{−y + 2z − 2v}{x}</td>
<td>\frac{4x + y − 2z + 2v}{8}</td>
<td>\frac{4x − y + 2z − 2v}{8}</td>
<td>(\frac{4x + y − 2z + 2v\cdot(4x − y + 2z − 2v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + HNO₂</td>
<td>+3</td>
<td>\frac{−y + 2z − 3v}{x}</td>
<td>\frac{4x + y − 2z + 3v}{8}</td>
<td>\frac{4x − y + 2z − 3v}{8}</td>
<td>(\frac{4x + y − 2z + 3v\cdot(4x − y + 2z − 3v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + NO₂</td>
<td>+4</td>
<td>\frac{−y + 2z − 4v}{x}</td>
<td>\frac{4x + y − 2z + 4v}{8}</td>
<td>\frac{4x − y + 2z − 4v}{8}</td>
<td>(\frac{4x + y − 2z + 4v\cdot(4x − y + 2z − 4v)}{8x})</td>
</tr>
<tr>
<td>C₆H₁₀N₂₅ + H₂O → CH₄ + CO₂ + HNO₃</td>
<td>+5</td>
<td>\frac{−y + 2z − 5v}{x}</td>
<td>\frac{4x + y − 2z + 5v}{8}</td>
<td>\frac{4x − y + 2z − 5v}{8}</td>
<td>(\frac{4x + y − 2z + 5v\cdot(4x − y + 2z − 5v)}{8x})</td>
</tr>
</tbody>
</table>
The ON in molecule \( \text{C}_x\text{H}_y\text{O}_z\text{N}_v \) matches the ON in the designated product. For example, when the \([\text{N-product}]\) is \( \text{HNO}_2 \) (ON = +3), the ON in molecule \( \text{C}_x\text{H}_y\text{O}_z\text{N}_v \) must equal to +3. With reference to Table 3, the relationships among AC, ON, \( \text{ON}_\text{C} \), SC, and \( \text{Te}^- \) in BEq are established. With any given structural formula of \( \text{C}_x\text{H}_y\text{O}_z\text{N}_v \), the \( \text{ON}_\text{C} \), \( n\text{CH}_4 \), \( n\text{CO}_2 \), and \( \text{Te}^- \) can be determined by the derived mathematical equations.

In summary, when ON_H = +1, ON_O = −2, and \( \Sigma\text{ON}_{\text{inc}} = (y - 2z + \text{ON}_N) \)

\[
\text{ON}_\text{C} = \frac{-\Sigma\text{ON}_{\text{inc}}}{x} = \frac{-(y-2z+\text{ON}_N)}{x}
\]

\[x \text{ ON}_\text{C} = -(y - 2z + \text{ON}_N)
\]

\[n\text{CH}_4 = \frac{4x+y-2z+\text{ON}_N}{8} = \frac{x(4-\text{ON_c})}{8}
\]

\[n\text{CO}_2 = \frac{4x-y+2z-\text{ON}_N}{8} = \frac{x(4+\text{ON_c})}{8}
\]

\[\text{Te}^- \text{ (oxidation)} = + \frac{(4x+y-2z+\text{ON}_N)(4x-y+2z-\text{ON}_N)}{8x} = + \frac{x(4-\text{ON_c})(4+\text{ON_c})}{8}
\]

The “+” sign represents there is a loss of electrons.

\[\text{Te}^- \text{ (reduction)} = - \frac{(4x+y-2z+\text{ON}_N)(4x-y+2z-\text{ON}_N)}{8x} = - \frac{x(4-\text{ON_c})(4+\text{ON_c})}{8}
\]

The “−” sign represents there is a gain of electrons.

\[\text{Te}^- = \frac{(4x+y-2z+\text{ON}_N)(4x-y+2z-\text{ON}_N)}{8x} = \frac{x(4-\text{ON_c})(4+\text{ON_c})}{8}
\]

When there is neither a “+” nor “−”, it represents the number of transferred electrons among organic carbons in overall BEqs.

7. From Counting \( \text{Te}^- \) to Balancing Buswell’s Equation for \( \text{C}_x\text{H}_y\text{O}_z\text{N}_v \) Molecules

The operating procedures for counting \( \text{Te}^- \) and balancing BEq are provided. In Examples 3, 4, and 5 (with reference to Eq1 and Eq2), the same empirical formula \( \text{C}_2\text{H}_5\text{O}_2\text{N} \) shows two different structural formulas \( \text{H}_2\text{N}^-\text{C}^-\text{C}^-\text{N}^+ \) and \( \text{H}_2\text{N}^-\text{C}^-\text{C}^-\text{N}^- \).

Example 3. Given \( \text{C}_2\text{H}_5\text{O}_2\text{N} \)

(a) Assign ON_{inc} and ON_C

\[
\begin{array}{|c|c|c|c|}
\hline
\text{Atom} & \text{C} & \text{H} & \text{O} & \text{N} \\
\hline
\text{ON}_{\text{inc}} & - & +1 & -2 & -3 \\
\text{AC} & 2 & 5 & 2 & 1 \\
\hline
\end{array}
\]

\[
\text{ON}_\text{C} = \frac{-\Sigma\text{ON}_{\text{inc}}}{x} = \frac{-(\text{ON}_\text{H} + \text{ON}_\text{O} + 2 + \text{ON}_\text{N})}{x}
\]

\[
= \frac{-(1+5+2+3)}{2} = +1
\]
(b) Determine \( n_{CH_4}, n_{CO_2}, \) and \( Te^- \)

<table>
<thead>
<tr>
<th>( x )</th>
<th>( ON_c )</th>
<th>( n_{CH_4} = \frac{x(4-ON_c)}{8} )</th>
<th>( n_{CO_2} = x - n_{CH_4} )</th>
<th>( Te^- = \frac{x(4-ON_c)(4+ON_c)}{8} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>+1</td>
<td>( n_{CH_4} = \frac{2[(4)-(1)]}{8} = \frac{3}{4} )</td>
<td>( n_{CO_2} = 2 - \frac{3}{4} = \frac{5}{4} )</td>
<td>( Te^- = \frac{2<a href="4+(1)">(4)-(1)</a>}{8} = \frac{15}{4} )</td>
</tr>
</tbody>
</table>

(c) Balance Macro-BEq

\[
\text{H}_2\text{N} \rightarrow \text{OH} + \text{nH}_2\text{O} \rightarrow \text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3
\]

Balance O atom:
\[
2 + \text{nH}_2\text{O} = \frac{5}{2}
\]
\[\text{nH}_2\text{O} = \frac{1}{2}\]

\[
\text{H}_2\text{N} \rightarrow \text{OH} + \frac{1}{2}\text{H}_2\text{O} \rightarrow \text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3, \text{Te}^- = \frac{15}{4}
\]

(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 equals \( \frac{15}{4} \).

Example 4. Given \((C_2H_5O_2N)\)

(a) Assign \( ON_{inc} \) and \( ON_c \)

<table>
<thead>
<tr>
<th>Atom</th>
<th>C</th>
<th>H</th>
<th>O</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ON_{inc} )</td>
<td>-</td>
<td>+1</td>
<td>-1</td>
<td>+3</td>
</tr>
<tr>
<td>( AC )</td>
<td>2</td>
<td>5</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

\[\text{ON}_c = \frac{-2ON_{inc}}{x} = \frac{-([ON_H y + ON_O z + ON_N v])}{x} = \frac{-[(+1)(5)+(-1)(2)+(+3)(1)]}{3} = -2\]

(b) Determine \( n_{CH_4}, n_{CO_2}, \) and \( Te^- \)

<table>
<thead>
<tr>
<th>( x )</th>
<th>( ON_c )</th>
<th>( n_{CH_4} = \frac{x(4-ON_c)}{8} )</th>
<th>( n_{CO_2} = x - n_{CH_4} )</th>
<th>( Te^- = \frac{x(4-ON_c)(4+ON_c)}{8} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-2</td>
<td>( n_{CH_4} = \frac{2[(4)-(-2)]}{8} = \frac{3}{2} )</td>
<td>( n_{CO_2} = 2 - \frac{3}{2} = \frac{1}{2} )</td>
<td>( Te^- = \frac{2<a href="4+(+2)">(4)-(-2)</a>}{8} = 3 )</td>
</tr>
</tbody>
</table>

(c) Balance Macro-BEq

\[
\text{H} \text{C} \text{N} \rightarrow \text{OH} + \text{nH}_2\text{O} \rightarrow \frac{3}{2}\text{CH}_4 + \frac{1}{2}\text{CO}_2 + \text{[N-product]}
\]
Identify \((ON_N = +3)\):

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

Balance \(N\) atom:

\[
\begin{align*}
\text{Reactants} & : & H^- + nH_2O & \rightarrow & \frac{3}{2}CH_4 + \frac{1}{2}CO_2 + HNO_2 \\
\text{Products} & : & H_2O & \rightarrow & 3CH_4 + \frac{1}{2}CO_2 + HNO_2
\end{align*}
\]

Balance \(O\) atom for counting \(nH_2O\):

\[
2 + nH_2O = 1 + 2 \quad \Rightarrow \quad nH_2O = 1
\]

\[
\begin{align*}
\text{Reactants} & : & H^- + H_2O & \rightarrow & \frac{3}{2}CH_4 + \frac{1}{2}CO_2 + HNO_2 ; Te^-= \frac{9}{2} \\
\text{Products} & : & \frac{1}{2}H_2O & \rightarrow & 3CH_4 + \frac{1}{2}CO_2 + HNO_2
\end{align*}
\]

(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 \(H\) and \(N\) cause different \(Te^-\) and \(CH_4\) \(nCO_2\) in \(n\) \(Te^-\) \(H\) \(O\) \(N\) in \(n\) \(Te^-\) \(C1\) for \(CH_4\) and \(C2\) for \(CO_2\) cause different \(Te^-\) and \(nCH_4\) \(nCO_2\) in \(Te^-\). In other words, they are two different \(n\) \(Beq\).

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 \(ON_{inc}\)

\[
\begin{array}{c|c|c|c|c|c}
\text{Reactants} & H & H & O^- & H_2O & \text{Products} \\
\hline
\text{Reactants} & CH_4 & CO_2 & NH_3 \\
\hline
ON_H = +1, ON_O = -2, ON_N = +3 & ON_H = +1, ON_O = -2, ON_N = +3 & ON_H = +1 & ON_O = -2 & ON_N = -3 \\
\hline
\end{array}
\]

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

\[
\begin{array}{c|c|c|c}
\text{Before the reaction} & \text{After the reaction} & \text{Change in } ON_{inc} \\
\hline
ON_H = +1 & ON_H = +1 & \Delta ON_H = 0 \\
ON_O = -2 & ON_O = -2 & \Delta ON_O = 0 \\
ON_N = +3 & ON_N = -3 & \Delta ON_N \neq 0 \\
\hline
\end{array}
\]

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

\[
\Sigma Te^- = Te^- (C1\text{ for } CH_4) + Te^- (C2\text{ for } CO_2) + Te^- (H) + Te^- (O) + Te^- (N)
\]

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

\[
\therefore \Delta ON_{C1} \neq 0, \Delta ON_{C2} \neq 0, \Delta ON_H = 0, \Delta ON_O = 0, \Delta ON_N \neq 0
\]
In summary:

\[ 0 = n\text{CH}_4 \Delta \text{ON}_{C1} + n\text{CO}_2 \Delta \text{ON}_{C2} + n\text{N} \Delta \text{ON}_{N} \]

Since \( \Delta \text{ON}_{N} = [(−3)−(+3)] = −6 < 0 \), the N atom (\( \text{ON}_{N} = +3 \)) gains electrons from organic carbons.

\[ 0 = n\text{CH}_4 \Delta \text{ON}_{C1} \text{ (gain of electrons)} + n\text{CO}_2 \Delta \text{ON}_{C2} \text{ (loss of electrons)} + n\text{N} \Delta \text{ON}_{N} \text{ (gain of electrons)} \]

\[ \Delta \text{Te}^- \text{ (reduction for CH}_4) \neq \Delta \text{Te}^- \text{ (oxidation for CO}_2) \]

Since there is electron transfer from carbon atoms (loss of electrons) to nitrogen atom (\( \Delta \text{ON}_{N} < 0; \text{gain of electrons} \)), \( \Delta \text{Te}^- \) (reduction for \( \text{CH}_4 \)) is not equal to \( \Delta \text{Te}^- \) (oxidation for \( \text{CO}_2 \)). Therefore, the given stoichiometric chemical equation

\[ (\text{C}_2\text{H}_5\text{O}_2\text{N})\frac{1}{2}\text{H}_2\text{O} \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3 \]

is not a BEq.

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

\[
\text{BEq-Ratio: } \frac{n\text{CH}_4}{n\text{CO}_2} = \frac{(4−\text{ON}_C)}{(4+\text{ON}_C)}
\]

<table>
<thead>
<tr>
<th>Structural formula (SF)</th>
<th>Balanced chemical equation (Eq)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \text{H} - \text{C} - \text{N}^- \text{O}^− ]</td>
<td>[ (\text{C}_2\text{H}_5\text{O}_2\text{N})\frac{1}{2}\text{H}_2\text{O} \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3 ]</td>
</tr>
</tbody>
</table>
| ON_C = −2 \[
\frac{(4−\text{ON}_C)}{(4+\text{ON}_C)} = \frac{4−(−2)}{4+(−2)} = 3
\] | nCH_4 = \(\frac{3}{4}\), nCO_2 = \(\frac{5}{4}\) |

Since the SF’s \( \frac{(4−\text{ON}_C)}{(4+\text{ON}_C)} (= 3) \) is not equal to the Eq’s \( \frac{n\text{CH}_4}{n\text{CO}_2} (= \frac{3}{5}) \), the Eq of \( (\text{C}_2\text{H}_5\text{O}_2\text{N})\frac{1}{2}\text{H}_2\text{O} \rightarrow \frac{3}{4}\text{CH}_4 + \frac{5}{4}\text{CO}_2 + \text{NH}_3 \) is not a BEq.

8. Deriving Mathematical Relationships in General Buswell’s Equation of \( \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t \)

The strategy above, which is used for balancing and deducing \( \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t \), can be extended to work on organic molecules which contain the formula \( \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t \). All possible \( \text{ON}_{\text{inc}} \) are: \( \text{ON}_H = +1 \text{ or } −1, \text{ON}_O = +1 \text{ or } −1, \text{ON}_X = \text{integers between } −1 \text{ and } +7, \text{ON}_N = \text{integers between } −3 \text{ and } +5, \text{ON}_S = \text{integers between } −2 \text{ and } +6, \text{and } \text{ON}_P = \text{integers between } −3 \text{ and } +5. \)

The unbalanced general BEQ equation is shown as:

\[ \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{CO}_2 + \text{[H-product]} + \text{[O-product]} + \text{[X-product]} + \text{[N-product]} + \text{[S-product]} + \text{[P-product]} \]

All \( \text{ON}_{\text{inc}} \) in \( \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t \) molecules remain the same before and after the reactions, therefore, \( \Delta \text{ON}_H = 0, \Delta \text{ON}_O = 0, \Delta \text{ON}_X = 0, \Delta \text{ON}_N = 0, \Delta \text{ON}_S = 0, \text{and } \Delta \text{ON}_P = 0. \)

With reference to Example 2, all \( \text{ON}_{\text{inc}}, \text{ON}_C, \text{SC}, \text{and } \Delta \text{Te}^- \) of \( \text{C}_n\text{H}_2\text{O}_x\text{N}_y\text{S}_z\text{P}_t \) in BEQ can be determined.

In summary:

\[ \text{ON}_C = \frac{−(\text{ON}_H y + \text{ON}_O z + \text{ON}_X w + \text{ON}_N v + \text{ON}_S u + \text{ON}_P t)}{x} \]

\[ n\text{CH}_4 = \frac{4x + (\text{ON}_H y + \text{ON}_O z + \text{ON}_X w + \text{ON}_N v + \text{ON}_S u + \text{ON}_P t)}{8} \]

\[ n\text{CO}_2 = \frac{4x − (\text{ON}_H y + \text{ON}_O z + \text{ON}_X w + \text{ON}_N v + \text{ON}_S u + \text{ON}_P t)}{8} \]

\[ \text{Te}^- = \frac{[4x + (\text{ON}_H y + \text{ON}_O z + \text{ON}_X w + \text{ON}_N v + \text{ON}_S u + \text{ON}_P t)] [4x − (\text{ON}_H y + \text{ON}_O z + \text{ON}_X w + \text{ON}_N v + \text{ON}_S u + \text{ON}_P t)]}{8x} \]
8.1 Relationships among $ON_C, ON_{inc}, nCH_4,$ and $nCO_2$

For $C_nH_{2n+1}O_xN_yS_zP_t$ molecules:

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

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

where $nC = x =$ number of organic carbons

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

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

8.2 Relationships among $Te^-$, $AC$, and $\Sigma ON_{inc}$

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

$$Te^- = \frac{4x + (ON_H y + ON_O z + ON_X w + ON_N v + ON_S u + ON_P t)}{8} \cdot \frac{4x + \Sigma ON_{inc}}{8}$$

8.3 Relationships among $Te^-$, $ON_C$, and $AC$

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

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

8.4 Relationships among $Te^-$, $ON_C$, $x$, $nCH_4$, and $nCO_2$

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

$$x = nCH_4 + nCO_2$$

$$nCO_2 = x - nCH_4$$

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

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

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

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

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

8.5 Relationships among $Te^-$, $ON_{inc}, ON_C, AC, nCH_4, nCO_2$

Mathematical equations for counting $Te^-$ of $C_nH_{2n+1}O_xN_yS_zP_t$ are summarized in Table 4. Relationships among $AC$, $ON_{inc}$, $ON_C$, $nCH_4$, $nCO_2$, and $Te^-$ are shown in Figure 2.
Table 4. Mathematical equations for counting Te\(^{-}\) of \(\text{C}_x\text{H}_y\text{O}_z\text{N}_w\text{S}_v\text{P}_t\) in BEq

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Mathematical equations for counting Te(^{-})</th>
</tr>
</thead>
<tbody>
<tr>
<td>AC, ON(_{\text{inc}})</td>
<td>(\text{Te}^{-} = \frac{[4x+(\text{ON}<em>\text{H}) + \text{ON}</em>\text{O} + \text{ON}<em>\text{N} + \text{ON}</em>\text{S} + \text{ON}_\text{P} + 1]}{8x} )</td>
</tr>
<tr>
<td>AC, ΣON(_{\text{inc}})</td>
<td>(\text{Te}^{-} = \frac{(4x - \Sigma\text{ON}<em>{\text{inc}})(4x + \Sigma\text{ON}</em>{\text{inc}})}{8x} )</td>
</tr>
<tr>
<td>ON(_{\text{C}}, x)</td>
<td>(\text{Te}^{-} = \frac{x(4-\text{ON}<em>\text{C})(4+\text{ON}</em>\text{C})}{8} )</td>
</tr>
<tr>
<td>nCH(<em>{4}), ON(</em>{\text{C}})</td>
<td>(\text{Te}^{-} = \text{nCH}<em>4 (4+\text{ON}</em>\text{C}))</td>
</tr>
<tr>
<td>nCO(<em>{2}), ON(</em>{\text{C}})</td>
<td>(\text{Te}^{-} = \text{nCO}<em>2 (4-\text{ON}</em>\text{C}))</td>
</tr>
<tr>
<td>nCH(<em>{4}), ON(</em>{\text{C}}, x)</td>
<td>(\text{Te}^{-} = (x-n\text{CH}<em>4)(4-\text{ON}</em>\text{C}))</td>
</tr>
</tbody>
</table>

Figure 2. Relationships among AC, ON\(_{\text{inc}}\), ON\(_{\text{C}},\) nCH\(_{4}\), nCO\(_{2}\), and Te\(^{-}\)

8.6 Relationships among ON\(_{\text{C}},\) Te\(^{-}\), and nCH\(_{4}\)

Based on the mathematical equations of \(\text{nCH}_4 = \frac{x(4-\text{ON}_\text{C})}{8} \) and \(\text{Te}^{-} = \frac{x(4-\text{ON}_\text{C})(4+\text{ON}_\text{C})}{8} \), \(\text{Te}^{-} = \text{nCH}_4 (4+\text{ON}_\text{C})\) is derived.

The triangular relationships among ON\(_{\text{C}},\) nCH\(_{4}\), and Te\(^{-}\) are shown in Figure 3.

Figure 3 Triangular relationships among ON\(_{\text{C}},\) 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 among ON\(_{\text{C}},\) 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 using the derived mathematical equations. The operating scheme is shown 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 \( ON_C \)

<table>
<thead>
<tr>
<th>Atom</th>
<th>C</th>
<th>H</th>
<th>O</th>
<th>N</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>ON</td>
<td>-</td>
<td>+1</td>
<td>-2</td>
<td>-3</td>
<td>+4</td>
</tr>
<tr>
<td>AC</td>
<td>2</td>
<td>7</td>
<td>3</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

\[
ON_C = \frac{-\sum ON_{inc}}{x} = \frac{-(ON_H + ON_O + ON_N + ON_S)}{x} = -1
\]

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

\[
\begin{array}{c|c|c|c|c|c}
 x & ON_C & nCH_4 = \frac{x(4+ON_C)}{8} & nCO_2 = x - nCH_4 & Te^- = nCH_4(4+ON_C) \\
\hline
 2 & -1 & \frac{2(4+(-1))}{8} = \frac{2}{4} & \frac{2 - \frac{2}{4}}{4} = \frac{3}{4} & \frac{2}{4}[4+(-1)] = \frac{10}{4}
\end{array}
\]

(c) Balance Macro-BEq

\[
\begin{align*}
\text{Balance O atom: } & 3 + nH_2O = \frac{3}{2} + 2 \\
nH_2O & = \frac{1}{2} \\
C_2H_7O_3NS + \frac{1}{2}H_2O & \rightarrow \frac{5}{4}CH_4 + \frac{3}{4}CO_2 + NH_3 + SO_2 \\
\text{Te}^- & = \frac{15}{4}
\end{align*}
\]

(d) Balance Micro-BEq

\[
4C_2H_7O_3NS + 2H_2O \rightarrow 5CH_4 + 3CO_2 + 4NH_3 + 4SO_2, \quad \text{Te}^- = 15
\]

(e) Draw BEq-Te⁻ diagram (disproportionation: 8C → 5C + 3C)
Example 7. Given Chlorthion, \( \text{C}_8\text{H}_9\text{O}_5\text{ClNSP} \):

(a) Assign ON\(_{\text{inc}}\) and ON\(_{C}\)

\[
\begin{array}{c|cccccccc}
\text{Atom} & \text{C} & \text{H} & \text{O} & \text{Cl} & \text{N} & \text{S} & \text{P} \\
\text{ON}\_{\text{inc}} & - & +1 & -2 & -1 & +3 & -2 & +5 \\
\text{AC} & 8 & 9 & 5 & 1 & 1 & 1 & 1 \\
\end{array}
\]

\[
\text{ON}_C = \frac{-(\text{ON}_\text{H} + \text{ON}_\text{O} + \text{ON}_\text{N} + \text{ON}_\text{Cl} + \text{ON}_\text{S} + \text{ON}_\text{P})}{x} \\
= \frac{-[(1)(9)+(-2)(5)+(-1)(1)+(3)(1)+(-2)(1)+(5)(1)]}{8} = -\frac{1}{2}
\]

(b) Determine nCH\(_4\), nCO\(_2\), and Te\(^-\)

\[
\begin{array}{c|c|c|c}
\text{x} & \text{ON}_C & \text{nCH}_4 & \text{nCO}_2 \\
8 & -\frac{1}{2} & \frac{8(4-(-\frac{1}{2}))}{8} = \frac{9}{2} & 8 - \frac{9}{2} = \frac{7}{2} \\
\end{array}
\]

\[
\text{Te}^- = \text{nCH}_4 (4+\text{ON}_C) \\
= (\frac{9}{2})(4+\frac{1}{2}) = \frac{63}{4}
\]

(c) Balance Macro-BEq

\[
\text{C}_8\text{H}_9\text{O}_5\text{ClNSP} + 8\text{H}_2\text{O} \rightarrow 9\text{CH}_4 + \frac{7}{2}\text{CO}_2 + \text{HCl} + \text{HNO}_2 + \text{H}_2\text{S} + \text{H}_3\text{PO}_4
\]

Balance O atom: 5 + 8\text{H}_2\text{O} = 7 + 2 + 4

\[
\text{nH}_2\text{O} = 8
\]

\[
\text{C}_8\text{H}_9\text{O}_5\text{ClNSP} + 8\text{H}_2\text{O} \rightarrow 9\text{CH}_4 + \frac{7}{2}\text{CO}_2 + \text{HCl} + \text{HNO}_2 + \text{H}_2\text{S} + \text{H}_3\text{PO}_4, \text{Te}^- = \frac{63}{4}
\]

(d) Balance Micro-BEq

\[
4\text{C}_8\text{H}_9\text{O}_5\text{ClNSP} + 32\text{H}_2\text{O} \rightarrow 18\text{CH}_4 + 14\text{CO}_2 + 4\text{HCl} + 4\text{HNO}_2 + 4\text{H}_2\text{S} + 4\text{H}_3\text{PO}_4, \text{Te}^- = 63
\]

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

\[
\begin{array}{c|c|c}
\text{32C} & 14\text{C} & 14\text{CH}_4 \\
& 63\text{e}^- & 18\text{CO}_2 \\
(14\text{C gain 63e}^-) & (18\text{C lose 63e}^-)
\end{array}
\]
10. Conclusions
By using ONc as a redox metric for BEq, the relationships among ONc, nCH4, nCO2, and Te− are established. The number of transferred electrons on organic carbons drives the disproportionation to the formations of CH4 to CO2 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) determine the Buswell-Ratio \( \frac{n\text{CH}_4}{n\text{CO}_2} = \frac{4-\text{ONc}}{4+\text{ONc}} \), (2) count Buswell-Electron by using \( \text{Te}^- = \frac{n(4-\text{ONc})(4+\text{ONc})}{8} \), \( \text{Te}^- = n\text{CH}_4 (4+\text{ONc}) \), or \( \text{Te}^- = n\text{CO}_2 (4-\text{ONc}) \), and (3) demonstrate 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.

Additional Information to Article

The below information will be added to the end of the above article.
Author(s) should replace the text in RED. If no information available, please write “Not applicable.”

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Authors contributions
P. K. Y. conceived and designed the idea. P. K. Y and C. M. D. L. wrote, reviewed, and edited the manuscript. All the authors discussed the results and commented on the manuscript.

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