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Empirical Buswell's Equation for Identifying Anaerobic Digestate

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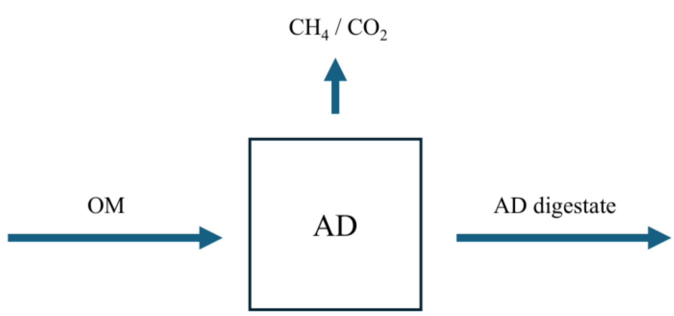
Abstract

Anaerobic digestion is a promising circular economic technology. Using organic matters as feedstocks, Buswell's equation can represent anaerobic digestion in accordance with the elemental composition of any organic matter. An organic feedstock is biodegradable to biomethane, biogenetic carbon dioxide, and digestate, but the management of anaerobic digestate encounters some environmental and technological challenges. Currently there is a research gap between Buswell's concept and the general organic elemental composition of unknown anaerobic digestate. To bridge the gap, this research developed an empirical Buswell's equation for identifying anaerobic digestate through the integration of theoretical Buswell's equation and experimental biomethane potential. This model can identify the organic elemental composition and characteristics of any anaerobic digestate, as well as reveal the correlation between an organic matter and its anaerobic digestate. It also discovers a higher heat value of anaerobic digestate which is greater than that of its corresponding organic matter. In addition, the empirical Buswell's equation can be used for assessing the validity of the empirical formula of organic feedstock.

Keywords: anaerobic digestion (AD), Buswell's equation for biomethane (BEq), empirical Buswell's equation for anaerobic digestate (empirical BEq), anaerobic digestate (AD digestate), higher heat value (HHV)

Graphical Abstract



Buswell's equation for Biomethane (BEq)

$$C_xH_yO_zX_wN_vS_uP_t \text{ (OM)} + nH_2O\ H_2O \rightarrow nCH_4\ CH_4 + nCO_2\ CO_2 + wHX + vNH_3 + uH_2S + tH_3PO_4$$

Buswell's equation for AD digestate (Empirical BEq)

$$C_xH_yO_zX_wN_vS_uP_t \text{ (OM)} \rightarrow \text{Exp-}nCH_4\ CH_4 + \text{Exp-}nCO_2\ CO_2 + C_aH_bO_cX_wN_vS_uP_t \text{ (AD digestate)}$$

1. Introduction

Anaerobic digestion (AD) is a biochemical process using organic matters (OM) such as organic wastes and biomasses as feedstocks under anaerobic microbial conditions. AD is a promising circular economic technology (Sun, 2023; Wu et al., 2022), which can be represented by Buswell's equation (BEq). When an empirical formula of OM is identified, the stoichiometric BEq (Buswell & Mueller, 1952; Boyle, 1977; Yuen & Lau, 2023) can be found and it is shown as follows:

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

BEq determines the quantitative amount of biomethane (nCH_4) and theoretical biomethane potential (TBMP) (Angelidaki & Sanders, 2004; Yuen & Lau, 2024a). Through a biomethane potential (BMP) test (Angelidaki et al., 2009), experimental biomethane potential (EBMP) can be measured. The biodegradability index (BDI%) (Nielfa et al., 2015) is defined as the percentage ratio of EBMP to TBMP. It can evaluate the biodegradable performance of OM shown in the following:

$$BDI\% = \frac{EBMP}{TBMP} \times 100\%$$

$$BDI = \frac{EBMP}{TBMP}$$

AD generates biomethane, biogenetic carbon dioxide, and anaerobic digestate (AD digestate), the third of which is the liquid and solid residues remaining after the AD of a biodegradable feedstock. Although AD digestate is widely used as a biofertilizer containing inorganic and organic ingredients, it is met with management, environmental, safety (Sipko & Ablieieva, 2024; Lamolinara et al., 2022), and technological challenges (Alengebawy et al., 2024; Romio et al., 2024). Digestate's composition is the key for optimization of digestate management (Möller & Müller, 2012), therefore, digestate can be used as feedstock to regenerate biomethane and biochemicals for sustainability and circular economy.

Compared to inorganic macronutrients and micronutrients, there is little information on the organic elemental composition of AD digestate. There is a research gap between Buswell's concept and the unexplored territory of digestate's general elemental composition. Based on Buswell's concept, this research establishes a new empirical BEq for AD digestate (empirical BEq) to bridge the gap. With this empirical BEq model, the research can achieve four aims: (i) to identify the organic elemental composition of digestate, (ii) to evaluate the characteristics of digestate, (iii) to estimate the higher heat value (HHV) of digestate, and (iv) to find out the correlation between a couple of OM feedstock and AD digestate.

2. Establishment of Empirical Buswell's Equation for AD Digestate

2.1 Buswell's Concept

BEq is the study of stoichiometry of anaerobic digestion for OM. BEq shows that all organic carbons are disproportionated to CH_4 and CO_2 under anaerobic conditions (Yuen & Lau, 2024b). The theoretical BEq is shown in the following:

$$C_xH_yO_zX_wN_vS_uP_t + nH_2O\ H_2O \rightarrow \text{Theo-}nCH_4\ CH_4 + \text{Theo-}nCO_2\ CO_2 + wHX + vNH_3 + uH_2S + tH_3PO_4$$

When the empirical formula of an OM is identified, the OM's parameters (μ, ONc, and x) and BEq's parameters (nCH_4, nCO_2, and TBMP) (Yuen et al., 2024c) can be determined. When the experimental EBMP is measured, the BDI% of OM can be determined.

2.2 Empirical BEq for AD Digestate

This research establishes a new stoichiometric chemical equation named empirical BEq. The OM (reactant), CH_4, CO_2, and AD digestate (products) are shown in the following established empirical BEq:

$$C_xH_yO_zX_wN_vS_uP_t\ (OM) \rightarrow \text{Exp-}nCH_4\ CH_4 + \text{Exp-}nCO_2\ CO_2 + C_aH_bO_cX_wN_vS_uP_t\ (AD\ digestate)$$

$C_xH_yO_zX_wN_vS_uP_t$ stands for empirical formula of OM

$C_aH_bO_cX_wN_vS_uP_t$ stands for empirical formula of AD digestate

Exp-nCH_4 stands for experimental quantity amount of biomethane

Exp-nCO_2 stands for calculated quantity amount of carbon dioxide

2.3 Theoretical BEq and Empirical BEq

BEq and experimental EBMP are integrated to identify the general elemental composition of AD digestate. The empirical BEq is set up to bridge OM ($C_xH_yO_zX_wN_vS_uP_t$) and AD digestate ($C_aH_bO_cX_wN_vS_uP_t$) using experimental Exp-nCH_4 and calculated Exp-nCO_2. Exp-nCH_4 can be counted by measured EBMP, then the calculated quantity amount of Exp-nCO_2 can be determined by Exp-nCH_4.

When an Exp-nCH_4 is found, Exp-nCO_2 can be counted by the relationship between two sets of ratios. Both the ratios, $\frac{\text{Theo-nCH}_4}{\text{Theo-nCO}_2}$ from BEq and $\frac{\text{Exp-nCH}_4}{\text{Exp-nCO}_2}$ from empirical BEq, are equal to $\frac{(4-\text{ONc})}{(4+\text{ONc})}$ (Yuen et al., 2024a). When Exp-nCH_4 is found, Exp-nCO_2 can then be counted.

Determine Exp-nCO_2

Theoretical BEq: $\frac{\text{Theo-nCH}_4}{\text{Theo-nCO}_2} = \frac{\text{nCH}_4}{\text{nCO}_2} = \frac{(4-\text{ONc})}{(4+\text{ONc})}$

Empirical BEq: $\frac{\text{Exp-nCH}_4}{\text{Exp-nCO}_2} = \frac{(4-\text{ONc})}{(4+\text{ONc})}$

$\because \frac{\text{Theo-nCH}_4}{\text{Theo-nCO}_2} = \frac{\text{Exp-nCH}_4}{\text{Exp-nCO}_2} \quad \therefore \text{Exp-nCO}_2 = \text{Exp-nCH}_4 \times \frac{\text{Theo-nCO}_2}{\text{Theo-nCH}_4} = \text{Exp-nCH}_4 \times \frac{(4+\text{ONc})}{(4-\text{ONc})}$

Consequently, the elemental composition of AD digestate ($C_aH_bO_cX_wN_vS_uP_t$) can be identified by the conservation of atoms.

Balance a general empirical BEq

$C_xH_yO_zX_wN_vS_uP_t \rightarrow \text{Exp-nCH}_4\ CH_4 + \text{Exp-nCO}_2\ CO_2 + C_aH_bO_cX_wN_vS_uP_t$

Balance C: $x = \text{Exp-nCH}_4 + \text{Exp-nCO}_2 + a$

Balance H: $y = 4(\text{Exp-nCH}_4) + b$

Balance O: $z = 2(\text{Exp-nCO}_2) + c$

Find $a = x - \text{Exp-nCH}_4 - \text{Exp-nCO}_2$, $b = y - 4(\text{Exp-nCH}_4)$, and $c = z - 2(\text{Exp-nCO}_2)$

3. Identifying AD Digestate

The working procedures for identifying AD digestate are as follows: (i) identify OM, (ii) find OM's parameters, (iii) count BEq's parameters, (iv) establish unbalanced empirical BEq, (v) determine empirical BEq, and (vi) attain balanced empirical BEq.

3.1 Data from Literature

Different OM samples of organic waste are retrieved from literature (Yasim & Buyong, 2023). The selected data of mass percentages of elements (mass%) and experimental EBMP are organized in Table 1.

Table 1. OM of organic waste: Mass% and EBMP

OM	C%	H%	O%	N%	S%	EBMP
CFW	46.29	8.16	33.66	7.35	0.54	328.39
UCFW	33.04	1.80	49.86	5.30	0.00	235.82
VW	43.62	6.45	31.56	5.21	0.16	209.12
FW	41.07	6.10	41.16	2.68	0.00	251.64
GW	40.79	5.31	39.32	1.59	0.00	274.94
PW	51.00	6.25	39.93	1.82	0.00	182.54
TW	76.30	3.63	17.86	0.21	0.00	174.02

3.2 Examples: Step-by-Step Procedure

Example 1. Based on the given mass% and EBMP of CFW in Table 1, (i) find OM's parameters: empirical formula mass (μ_{OM}), empirical formula, mean oxidation number of organic carbons (ONc), and x, (ii) determine BEq's parameters:

nCH_4, TBMP, and BDI%, (iii) attain BEq, (iv) establish empirical BEq for AD digestate, and (v) identify elemental composition of digestate $C_aH_bO_cN_vS_u$

Step 1. Find OM's parameter: empirical formula, μ_{OM}, ONc, and x (Yuen et al., 2024c)

C%	H%	O%	N%	S%	$\mu_{OM} = \sum$mass%	Empirical formula of CFW	ONc = $\frac{-y+2z+3v+2u}{x}$	x
46.29	8.16	33.66	7.35	0.54	96.00	$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$	–0.591	3.854

Step 2. Determine BEq's parameters: nCH_4, nCO_2, and $\frac{nCH_4}{nCO_2}$

$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$ + nH_2O H_2O → nCH_4 CH_4 + nCO_2 CO_2 + $0.525NH_3$ + $0.017H_2S$

$nCH_4 = \frac{x(4-ONc)}{8}$	$nCO_2 = x - nCH_4$	$\frac{nCH_4}{nCO_2}$
$= \frac{3.854[4-(-0.591)]}{8}$ = 2.212	= 3.854 – 2.212 = 1.642	$= \frac{2.212}{1.642}$ = 1.347

Step 3. Attain the balanced BEq

$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$ (OM) + nH_2O H_2O → $2.212CH_4$ + $1.642CO_2$ + $0.525NH_3$ + $0.017H_2S$

Balance O: $2.104 + nH_2O = 2(1.642)$

$nH_2O = 1.180$

The balanced BEq is $C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$ (OM) + $1.180H_2O$ → $2.212CH_4$ + $1.642CO_2$ + $0.525NH_3$ + $0.017H_2S$

Step 4. Identify BEq's parameters: TBMP and BDI%

TBMP = $\frac{22400\ (nCH_4)}{\mu OM}$	Measured EBMP	BDI% = $\frac{EBMP}{TMBP}$ × 100%
$= \frac{22400\ (2.212)}{96.00}$ = 516.133	(328.39)	$= \frac{(328.39)}{516.133}$ × 100% = 63.63%

Step 5. Set up unbalanced empirical BEq for AD digestate

$C_xH_yO_zN_vS_u$ (OM) → Exp-nCH_4 CH_4 + Exp-nCO_2 CO_2 + $C_aH_bO_cN_vS_u$ (AD digestate)
$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$ → Exp-nCH_4 CH_4 + Exp-nCO_2 CO_2 + $C_aH_bO_cN_{0.525}S_{0.017}$

Step 6. Determine the stoichiometric coefficients of empirical BEq: Exp-nCH_4 and Exp-nCO_2

Exp-$nCH_4 = \frac{\mu\ (EBMP)}{22400}$	$\frac{nCH_4}{nCO_2}$ (from BEq)	$\frac{nCO_2}{nCH_4}$	Exp-nCO_2 = Exp-nCH_4 $(\frac{nCO_2}{nCH_4})$
$= \frac{96.00\ (328.39)}{22400}$ = 1.407	$= \frac{2.212}{1.642}$ = 1.347	$= \frac{1}{1.347}$	$= 1.407\ (\frac{1}{1.347})$ = 1.045

Step 7. Identify the elemental composition of $C_aH_bO_cN_vS_u$: by conservation of atoms

Balanced empirical BEq:

$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$ → $1.407CH_4$ + $1.045CO_2$ + $C_aH_bO_cN_{0.525}S_{0.017}$

Balance C: $3.854 = 1.407 + 1.045 + a$

Balance H: $8.095 = 4(1.407) + b$

Balance O: $2.104 = 2(1.045) + c$

Find a = 1.402, b = 2.467, and c = 0.014

The elemental composition of AD digestate is identified as $C_{1.402}H_{2.467}O_{0.014}N_{0.525}S_{0.017}$

Step 8. Attain balanced empirical BEq

$$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017} \rightarrow 1.407CH_4 + 1.045CO_2 + C_{1.402}H_{2.467}O_{0.014}N_{0.525}S_{0.017}$$

By the above working strategy, the calculated data of OM's parameters and BEq's parameters for OM (Table 1) are summarized in Table 2a and 2b. The calculated data of AD digestates are summarized in Table 3a and 3b.

Table 2a. Empirical formula of OM and OM's parameters

OM	μ	nC	nH	nO	nN	nS	ONc	EF
CFW	96.00	3.854	8.095	2.104	0.525	0.017	-0.591	$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$
UCFW	90.00	2.751	1.786	3.116	0.378	0.000	2.029	$C_{2.751}H_{1.786}O_{3.116}N_{0.378}$
VW	87.00	3.632	6.399	1.973	0.372	0.005	-0.366	$C_{3.632}H_{6.399}O_{1.973}N_{0.372}S_{0.005}$
FW	91.01	3.419	6.052	2.573	0.191	0.000	-0.097	$C_{3.419}H_{6.052}O_{2.573}N_{0.191}$
GW	87.01	3.396	5.268	2.458	0.114	0.000	-0.004	$C_{3.396}H_{5.268}O_{2.458}N_{0.114}$
PW	99.00	4.246	6.200	2.496	0.130	0.000	-0.193	$C_{4.246}H_{6.200}O_{2.496}N_{0.130}$
TW	98.00	6.353	3.601	1.116	0.015	0.000	-0.208	$C_{6.353}H_{3.601}O_{1.116}N_{0.015}$

Table 2b. OM's parameters and BEq's parameters

OM	x = nC	μ	ONc	nCH_4	nCO_2	$\frac{nCH_4}{nCO_2}$	TBMP	EBMP	BDI%
CFW	3.854	96.00	-0.591	2.212	1.642	1.347	516.117	328.39	63.63
UCFW	2.751	90.00	2.029	0.678	2.073	0.327	168.651	235.82	139.83
VW	3.632	87.00	-0.366	1.982	1.650	1.201	510.256	209.12	40.98
FW	3.419	91.01	-0.097	1.751	1.668	1.050	431.021	251.64	58.38
GW	3.396	87.01	-0.004	1.700	1.697	1.002	437.529	274.94	62.84
PW	4.246	99.00	-0.193	2.225	2.021	1.101	503.532	182.54	36.25
TW	6.353	98.00	-0.208	3.342	3.011	1.110	763.818	174.02	22.78

The difference between calculated TBMP of CFW in Example 1 (516.133 mL/g) and TBMP of CFW in Table 2b (516.117 mL/g) is due to rounding numbers in calculation.

Table 3a. AD digestate's parameters **(**$C_aH_bO_cN_vS_u$**)**

AD digestate	a	b	c	v	u	μ	ONc
CFW	1.402	2.465	0.014	0.525	0.017	27.450	-0.591
UCFW	-1.094	-2.004	-2.679	0.378	0.000	-52.728	2.029
VW	2.144	3.150	0.620	0.372	0.005	44.219	-0.365
FW	1.423	1.962	0.626	0.191	0.000	31.752	-0.097
GW	1.262	0.996	0.326	0.114	0.000	22.982	-0.001
PW	2.706	2.973	1.030	0.130	0.000	53.812	-0.193
TW	4.906	0.556	-0.256	0.015	0.000	55.601	-0.208

Table 3b. Empirical formula of AD digestate and stoichiometric coefficients of empirical BEq

AD digestate	Empirical formula	Exp-nCH_4	Exp-nCO_2
CFW	$C_{1.402}H_{2.465}O_{0.014}N_{0.525}S_{0.017}$	1.407	1.045
UCFW	$C_{-1.094}H_{-2.004}O_{-2.679}N_{0.378}$	0.947	2.898
VW	$C_{2.144}H_{3.150}O_{0.620}N_{0.372}S_{0.005}$	0.812	0.676
FW	$C_{1.423}H_{1.962}O_{0.626}N_{0.191}$	1.022	0.974
GW	$C_{1.262}H_{0.996}O_{0.326}N_{0.114}$	1.068	1.066
PW	$C_{2.706}H_{2.973}O_{1.030}N_{0.130}$	0.807	0.733
TW	$C_{4.906}H_{0.556}O_{-0.256}N_{0.015}$	0.761	0.686

3.3 Empirical BEq as a Tool for Assessing the Validity of OM's Empirical Formula

In table 3b, the atomic coefficients (a, b, or c) of AD digestate ($C_{-1.094}H_{-2.004}O_{-2.679}N_{0.378}$) and ($C_{4.906}H_{0.556}O_{-0.256}N_{0.015}$) from OM feedstocks UCFW and TW were identified as negative values and are therefore invalid. With reference to Table 2a, the abnormal high molar ratio values of C/H = 1.540 for UCFW ($C_{2.751}H_{1.786}O_{3.116}N_{0.378}$) and C/H = 1.764 for TW ($C_{6.353}H_{3.601}O_{1.116}N_{0.015}$) are found due to the invalidity of the mass%. Those two sets of data will be eliminated in the following stages.

The experimental mass% are critical in the identification of empirical formula of organic feedstock and application of BEq. Through the step-by-step procedures, this article shows that when negative value of atomic coefficients (a, b, c) is shown in the empirical formula of AD digestate, the formula is invalid. The empirical formula of OM is invalid because the C/H ratio of its corresponding mass% is invalid. Critically, the empirical BEq model can be used to estimate the validity of both the C/H ratio of the empirical formula of OM and its corresponding mass%.

4. Characteristics of AD Digestate

AD digestate is composed of liquid and solid residues. When the theoretical elemental composition of AD Digestate $C_aH_bO_cN_vS_u$ is identified, its characteristics can be assessed.

4.1 Higher Heat Value (HHV)

HHV is generally used to represent the energy content of substance. Both the HHV of AD digestate and OM are counted by the modified Dulong formula (Channiwala & Parikh, 2002) and it is shown as:

$$HHV\ (KJ/kg) = 337[C] + 1419([H] - 1/8\ [O]) + 23.26[N] + 93[S]$$

where [C], [H], [O], [N], and [S] stand for mass % of C, H, O, N, and S elements

4.2 Determination of ONc, $\frac{nC}{\mu}$, TBMP, and HHV

With reference to Tables 2a/2b and 3a/3b, the calculated ONc, $\frac{nC}{\mu}$, TBMP, HHV of OM and AD digestate are counted and summarized in Tables 4 and 5 respectively.

Table 4. OM: calculated ONc, $\frac{nC}{\mu}$, TBMP, and HHV

OM	Empirical formula	ONc	nC = x	μ_{OM}	$\frac{nC}{\mu}$	TBMP	HHV
CFW	$C_{3.854}H_{8.095}O_{2.104}N_{0.525}S_{0.017}$	-0.591	3.854	96.00	0.040	516.117	21429.51
VW	$C_{3.632}H_{6.399}O_{1.973}N_{0.372}S_{0.005}$	-0.366	3.632	87.00	0.042	510.256	18390.60
FW	$C_{3.419}H_{6.052}O_{2.573}N_{0.191}$	-0.097	3.419	91.01	0.038	431.021	15258.07
GW	$C_{3.396}H_{5.268}O_{2.458}N_{0.114}$	-0.004	3.396	87.01	0.039	437.529	14343.72
PW	$C_{4.246}H_{6.200}O_{2.496}N_{0.130}$	-0.193	4.246	99.00	0.043	503.532	19015.50

Table 5. AD digestate: calculated ONc, $\frac{nC}{\mu}$, TBMP, and HHV

AD digestate	Empirical formula	ONc	nC = a	$\mu_{AD\ digestate}$	$\frac{nC}{\mu}$	TBMP	HHV
CFW	$C_{1.402}H_{2.465}O_{0.014}N_{0.525}S_{0.017}$	-0.591	1.402	27.450	0.051	656.379	34176.51
VW	$C_{2.144}H_{3.150}O_{0.620}N_{0.372}S_{0.005}$	-0.365	2.144	44.219	0.048	592.523	26137.32
FW	$C_{1.423}H_{1.962}O_{0.626}N_{0.191}$	-0.097	1.423	31.752	0.045	514.088	21583.72
GW	$C_{1.262}H_{0.996}O_{0.326}N_{0.114}$	-0.001	1.262	22.982	0.055	615.296	24562.26
PW	$C_{2.706}H_{2.973}O_{1.030}N_{0.130}$	-0.193	2.706	53.812	0.050	590.465	22904.56

4.3 Comparing a Couple of OM and AD Digestate

The characteristics of AD digestate can be understood by comparing any couple of OM and its AD digestate. The fixed ratio of Exp-nCH_4 and Exp-nCO_2, and AD digestate are produced by OM, therefore, a couple of OM and AD digestate should have the same ONc. The slight difference between OM-ONc (Table 4) and AD digestate-ONc (Table 5) is due to rounding numbers in calculation. Based on Tables 4 and 5, the values of nC and μ of OM are bigger than that of AD digestate, and the values of $\frac{nC}{\mu}$, TBMP, and HHV of OM are smaller than that of AD digestate. Table 6 compares the characteristics of OM and its corresponding AD digestate.

Table 6. Characteristics of OM ($C_xH_yO_zX_wN_vS_uP_t$) and its corresponding AD digestate ($C_aH_bO_cX_wN_vS_uP_t$)

Parameter	OM	vs	AD digestate
	$C_xH_yO_zX_wN_vS_uP_t$		$C_aH_bO_cX_wN_vS_uP_t$
ONc	ONc-OM	=	ONc-AD digestate
nc	nc-OM = x	>	nc-AD digestate = a
μ	μ_{OM}	>	$\mu_{AD\ digestate}$
$\frac{nc}{\mu}$	$\frac{x}{\mu OM}$	<	$\frac{a}{\mu AD\ digestate}$
TBMP	TBMP-OM	<	TBMP- AD digestate
HHV	HHV-OM	<	HHV-AD digestate

4.4 Sustainable Utilization of AD Digestate

The greater values of HHV and TBMP the AD digestate has, the greater feedstock potential the AD digestate possesses. Figure 2 shows the utilization of AD digestate as a regenerated feedstock for the second sustainable process (Algapani et al., 2019; Li et al., 2017; Dimotta & Freda, 2023).

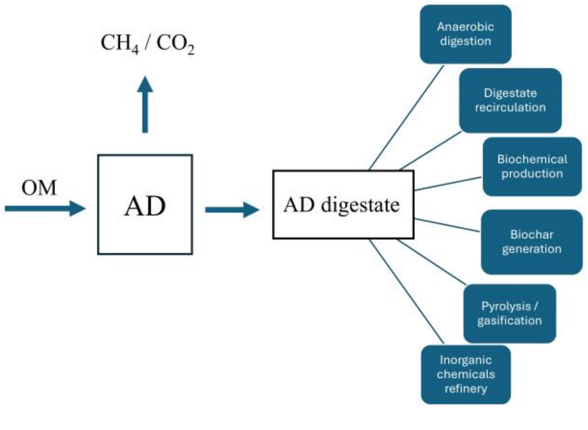


Figure 2. AD Digestate and 2nd stage process

5. Conclusion

The empirical BEq for AD digestate is established through the integration of theoretical Buswell's concept and experimental EBMP. The established empirical BEq model: (1) identifies the elemental composition of AD digestate, (2) reveals the characteristics between OM and its AD digestate, and (3) finds out that the AD digestate possesses higher HHV than its corresponding OM. In addition, through the step-by-step procedures, the empirical BEq model can determine the validity of OM's empirical formula.

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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. Kuok In Gabriel Yuen is responsible for data processing and figures drawing. All authors read and approved of the final manuscript.

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

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Obtained.

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Data availability statement

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

Data sharing statement

No additional data are available.

References

Alengebawy, A., Ran, Y., Osman, A. I., Jin, K., Samer, M., & Ping Ai, P. (2024). Anaerobic digestion of agricultural waste for biogas production and sustainable bioenergy recovery: a review. *Environmental Chemistry Letters, 22*(6), 2641-2668. https://doi.org/10.1007/s10311-024-01789-1

Algapani, D. E., Qiao, W., Marina Ricci, M., Davide Bianchi, D., M. Wandera, S. M., Adani, F., & Dong, R. (2019). Bio-hydrogen and bio-methane production from food waste in a two-stage anaerobic digestion process with digestate recirculation. *Renewable Energy, 130*, 1108-1115. https://doi.org/10.1016/j.renene.2018.08.079

Angelidaki, I., & Sanders, W. (2004). Assessment of the anaerobic biodegradability of macropollutants. *Reviews in Environmental Science and Biotechnology, 3*(2), 117-129. https://doi.org/10.1007/s11157-004-2502-3

Angelidaki, I., Alves, M., Bolzonella, D., Borzacconi, L., Campos, J. L., Guwy, A. J., … & van Lier, J. B. (2009). Defining the biomethane potential (BMP) of solid organic wastes and energy crops: a proposed protocol for batch assays. *Water Sci Technol, 59*(5), 927-934. https://doi.org/10.2166/wst.2009.040

Boyle, W. C. (1977). Energy recovery from sanitary landfills. Edited by Schlegel, H. G. & Barnea, J, In: *Microbial Energy Conversion,* 119-138. https://doi.org/10.1016/B978-0-08-021791-8.50019-6

Buswell, A. M., & Mueller, H. F. (1952). The mechanism of methane fermentation. *Industrial & Engineering Chemistry, 44*(3), 550-552. https://doi.org/10.1021/ja01185a034

Channiwala, S. A., & Parikh. P. P. (2002). A unified correlation for estimating HHV of solid, liquid and gaseous fuels. *Fuel, 81*(8), 1051-63. https://doi.org/10.1016/S0016-2361(01)00131-4

Dimotta, A., & Freda, C. (2023). Thermodynamic analysis of digestate pyrolysis coupled with CO_2 sorption. *Lecture Notes in Computer Science, 14111*, 150-161. https://doi.org/10.1007/978-3-031-37126-4_11

Lamolinara, B., Pérez-Martínez, A., Guardado-Yordi, E., Fiallos, C. G., Diéguez-Santana, K., Gerardo J., & Ruiz-Mercado, G. (2022). Anaerobic digestate management, environmental impacts, and techno-economic challenges. *Waste Management, 140,* 14-30. https://doi.org/10.1016/j.wasman.2021.12.035

Li, B., Yang, H., Wei, L., Shao, J., Wang, X., & Chen, H. (2017). Hydrogen production from agricultural biomass wastes gasification in a fluidized bed with calcium oxide enhancing. *International Journal of Hydrogen Energy, 42*(8), 4832-4839. https://doi.org/10.1016/j.ijhydene.2017.01.138

Möller, K., & Müller, T. (2012). Effects of anaerobic digestion on digestate nutrient availability and crop growth: A review. *Engineering in Life Sciences, 12*(3), 242-257. https://doi.org/10.1002/elsc.201100085

Nielfa, A., Cano, R., & Fdz-Polanco, M. (2015). Theoretical methane production generated by the co-digestion of organic fraction municipal solid waste and biological sludge. *Biotechnol. Rep., 5*(1), 14-21. https://doi.org/10.1016/j.btre.2014.10.005

Romio, C., Ward, A. J., & Møller, H. B. (2024) Characterization and valorization of biogas digestate and derived organic fertilizer products from separation processes. *Front. Sustain. Food Syst., 8*, 1415508. https://doi.org/10.3389/fsufs.2024.1415508

Sipko, I., & Ablieieva, I. (2024). Systematic approach to the formation of quality and environmental safety of biofertilizer from digestate. *Environmental Problems, 9*(3), 123-135. https://doi.org/10.23939/ep2024.03.123

Sun, D. (2023). Circular economy and municipal solid waste management in China. *Journal of Education Humanities* an*d Social Sciences, 8*, 1756-1762. https://doi.org/10.54097/ehss.v8i.4576

Wu, F., Li, F., Zhao, X., Bolan, N. S., Fu, P., Lam, S. S., … & Wang, H. (2022). Meet the challenges in the "Carbon Age". *Carbon Research, 1*, 1. https://doi.org/10.1007/s44246-022-00001-9

Yasim, S. E. M., & Buyong, F. (2023). Comparative of experimental and theoretical biochemical methane potential generated by municipal solid waste. *Environmental Advances, 11,* 100345. https://doi.org/10.1016/j.envadv.2023.100345

Yuen, P. K., & Lau, C. M. D. (2023). Using Buswell's equation to count quantity of biomethane in organochlorine compounds. *International Journal of Chemistry, 15*(2), 34-49. https://doi.org/10.5539/ijc.v15n2p34

Yuen, P. K., & Lau, C. M. D. (2024a). Using mean oxidation number of organic carbons to quantify Buswell's equation. *International Journal of Chemistry, 16*(1), 41-56. https://doi.org/10.5539/10.5539/ijc.v16n1p41

Yuen, P. K., & Lau, C. M. D. (2024b) Counting and demonstrating electron transfer in Buswell's equation. *International Journal of Chemistry, 16*(2), 42-61. https://doi.org/10.5539/ijc.v16n2p42

Yuen, P. K., Lau, C. M. D., & Yuen, K. I. G. (2024c). Calculations reconsidered: from mass percentages of elements to empirical formula and from empirical formula to theoretical biomethane potential. *International Journal of Chemistry, 16*(2), 75-86. https://doi.org/10.5539/ijc.v16n2p75