

Aerobic and Energy-Recovery Treatment Processes of Sanitary Waste to Reduce End-of-Life Carbon Emissions

Supplementary Information (S2) Reproducibility of the Stoichiometric Method

This document provides a reproducible, step-by-step derivation of the stoichiometric calculations used to obtain the emission yields reported in Table 3C, using the empirical formulas (Table 3B), the stoichiometric Equations (4) and (5), and the wet-dry basis of the functional unit (FU).

Algebraic development

S2.1 Functional unit and wet-dry basis

All yields and emission factors are reported per functional unit (FU):

- FU = 1 tonne of sanitary waste (SW), wet basis.

The wet-to-dry basis used for all calculations is:

- $M_{\text{wet}} = 1000 \text{ kg}$
- $M_{\text{dry}} = 902.2 \text{ kg}$
- $M_{\text{water}} = M_{\text{wet}} - M_{\text{dry}} = 97.8 \text{ kg}$

Moisture content on a wet basis is:

$$MC = \frac{M_{\text{water}}}{M_{\text{wet}}}$$

This FU basis is used consistently for Table 3C yields and for annual scaling in the main manuscript.

S2.2 Definition of “moles of substrate per FU” and mass-basis scaling

To reproduce the yields exactly as reported in Table 3C. We make explicit the conversion from “per mole of empirical substrate” to “per FU (1 t wet SW)”. The spreadsheet uses a mass-basis scaling based on the dry organic mass available for reaction, rather than assuming an arbitrary number of empirical-substrate moles.

S2.2.1 Dry organic mass available for reaction

Let f_{ash} be the ash fraction on a dry basis. Then the dry organic mass available for reaction is:

$$M_{OD} = M_{\text{dry}} (1 - f_{\text{ash}})$$

This is the mass that is treated as reactive organic material for stoichiometric conversion. Traceability note: all empirical formula coefficients (a, b, c, d, e) are taken from Table 3B, and the FU wet–dry basis (M_{wet} and M_{dry}) is taken from Table 3A / the spreadsheet implementation.

S2.2.2 Total reactant mass per “mole of substrate”

For each pathway, the spreadsheet defines a “total reactant mass per mole” on the reactant side (M_{total}), which is used as the denominator to scale product masses to the FU.

Aerobic case:

M_{total} is taken as the molar mass of the empirical substrate:

$$M_{total} = MW(C_a H_b O_c N_d)$$

Anaerobic case:

The Buswell-type reaction includes a stoichiometric water term on the reactant side. In the spreadsheet scaling, the “total reactant mass per mole” is taken as substrate plus stoichiometric water:

$$M_{total} = MW(C_a H_b O_c N_d S_e) + \nu_{H_2O} MW_{H_2O}$$

S2.2.3 Conversion of product masses to the FU

Once the product mass per mole of substrate is computed (from stoichiometric coefficients and molar masses), the spreadsheet scales to FU using:

$$m_{gas,FU} = \left(\frac{m_{gas,mol}}{M_{total}} \right) M_{OD}$$

Finally, yields reported in Table 3C (wet basis) are:

$$Y_{gas} = \frac{m_{gas,FU}}{M_{wet}} \text{ (reported as t t}^{-1} \text{ SW)}$$

This makes the pathway from empirical formula → stoichiometric coefficients → product mass per mole → FU-scaled mass explicit and identical to the spreadsheet audit trail.

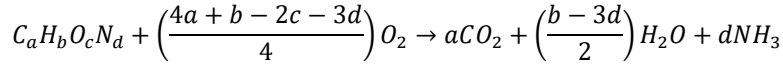
Table S2. Parameter definitions and units (for reproducibility)

Symbol	Definition	Units / basis
M_{wet}	Mass of sanitary waste in the functional unit (wet basis)	kg per FU (1000 kg)
M_{dry}	Dry mass associated with the FU	kg per FU
M_{water}	Water mass in the FU ($M_{wet} - M_{dry}$)	kg per FU
MC	Moisture content on wet basis (M_{water}/M_{wet})	–
f_{ash}	Ash mass fraction on dry basis	– (dry basis)
MOD	Dry organic mass available for reaction = $M_{dry}(1 - f_{ash})$	kg per FU
a, b, c, d, e	Empirical coefficients in $CaHbOcNdSe$ (from Table 3B)	–
ν_i	Stoichiometric coefficient of species (i) from Eqs. (4)–(5)	mol per mol

Symbol	Definition	Units / basis
		substrate
$m_{gas,mol}$	Gas mass per mole of substrate ($v_{gas} \cdot MW_{gas}$)	g mol ⁻¹ substrate
M_{total}	Total reactant-side mass per mole used for scaling (substrate; or substrate + $v_{H_2O} \cdot MW_{H_2O}$ in anaerobic case)	g per mol substrate
$m_{gas,FU}$	Gas mass per FU via mass-basis scaling ($m_{gas,mol}/M_{total}$) · M_{OD}	kg per FU
Y_{gas}	Yield reported ($m_{gas,FU}/M_{wet}$)	t t ⁻¹ SW (wet basis)

S2.3 Aerobic pathway (Eq. 4): coefficients and gas yields (general)

The aerobic oxidation pathway is represented by Eq. (4):



From Eq. (4), the principal stoichiometric coefficients are:

- CO₂ produced: $v_{CO_2} = a$
- Water produced: $v_{H_2O} = \frac{b-3d}{2}$
- Oxygen consumed: $v_{O_2} = \frac{4a+b-2c-3d}{4}$

The CO₂ mass produced per mole of substrate is:

$$m_{CO_2,mol} = v_{CO_2} MW_{CO_2}$$

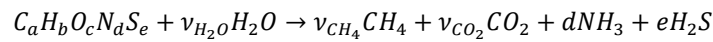
For the aerobic pathway, methane formation is assumed negligible:

$$m_{CH_4,mol} = 0$$

FU-scaled product masses and yields are obtained using the scaling in Section S2.2.

S2.4 Anaerobic pathway (Eq. 5): coefficients and gas yields (general)

The anaerobic conversion is represented as a Buswell-type relationship including N and S:



with:

$$\begin{aligned} v_{H_2O} &= a - \frac{b}{4} - \frac{c}{2} + \frac{3d}{4} + \frac{e}{2} \\ v_{CH_4} &= \frac{a}{2} + \frac{b}{8} - \frac{c}{4} - \frac{3d}{8} - \frac{e}{4} \\ v_{CO_2} &= \frac{a}{2} - \frac{b}{8} + \frac{c}{4} + \frac{3d}{8} + \frac{e}{4} \end{aligned}$$

Masses per mole of substrate are:

$$m_{CH_4,mol} = v_{CH_4} MW_{CH_4}$$

$$m_{CO_2, mol} = \nu_{CO_2} MW_{CO_2}$$

FU-scaled masses and yields follow Section S2.2.