Sustainable Valorisation of Agri-food Waste from Open-Air Markets in Kampala, Uganda via Standalone and Integrated Waste Conversion Technologies

Supplementary Information

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**Supplementary Information**

**SI-1 Integrative Assessment Modelling Approach**

Material Flow Analysis (MFA) is a mass balance approach for designing, characterising, and quantitatively assessing resource flows (from inputs to outputs, including emissions and accumulations retained) within a waste/waste-to-energy management system (WMS), providing evidence to support strategic interventions/sustainability targets. The types of material resource flow enabled by the MFA analysis include ‘goods’ (i.e., entities' economic value, e.g., residues, by-products) and ‘substances’ (i.e., chemical elements, such as heavy metals) [1]. Previous studies [2, 3] have shown that deploying MFA at ‘goods’, and ‘substances’ levels provides evidence to assess the magnitude of resource flow rates and hence the potential capacities of a WMS. Additionally, this enables the evaluation of the functionalities and performance of interlinked processes behind the metabolism of specific chemical elements (and emissions) within a WMS that could be of economic value or represent a hazardous risk to health and the environment. This purports substance flow analysis is critical from economic and environmental perspectives, enabling adequate resource recovery and plugging hazardous substances into the environment. However, while MFA enables the identification and quantification of resource flow within a WMS, it is limited because it does not provide an understanding of the likely environmental impact assessments associated with the flows, especially potentially hazardous *‘goods’,* and *‘substances’*. In this respect, the Life Cycle Analysis (LCA), a distinguished assessment tool for quantifying and categorising environmental impacts, provides short, medium, and long-term impacts of processes and resource flow (e.g., hazardous substances) throughout their life cycle to enable a comprehensive and holistic assessment. Further, optimised inputs, outputs, and operating parameters enabled by waste-to-energy process modelling & simulation provide theoretical evidence of the performance and efficiencies of conversion processes for WMS planning and implementation [4, 5]. Integrating MFA, LCA, and waste-to-energy process modelling thus provides a rigorous scientific basis for comparative evaluation of performance, resource recovery and environmental impact assessment of technology-based solutions for managing agri-food waste, in this study, from open-air markets.

**SI-2 Agri-food waste characterisations and analyses**

|  |  |  |  |
| --- | --- | --- | --- |
| Properties | Parameters | Analytical techniques/ equipment | Standard Methods Reference |
| Physical | Moisture content, MC | Thermogravemetric analyser | APHA (2005) [6] |
| Total solids, TS | Drying method, (Dried at 105°C) |
| Volatile solids, VS | Thermogravemetric analyser |
| Ash content |
| pH | pH probe |
| Biochemical | COD | Closed reflux and colorimetric measurement |
| Metals: Ca, Na, Fe, Mn, Zn, K, Mg, Cd, Cr, Cu, Ni, Pb | Digestion and AAS-graphite furnace |
| Metals: As, Hg | Digestion and AAS-Hydride |
| Ultimate analyses – C, H, N, S, O | Elemental analyzer | ASTM D5373 |
| Energy | Calorific value (HHV) | Bomb calorimeter | ISO 1928:2009 |
| Bromatological | Carbohydrates | Proximate analyser |  |
| Protein content | Proximate analysis |
| Lipids |  |

**SI-3 Process simulation modelling - Simplified flow diagrams**

Diagram

Description automatically generated with medium confidence

Figure SI-3a Simplified process flow model for S2\_AD scenario

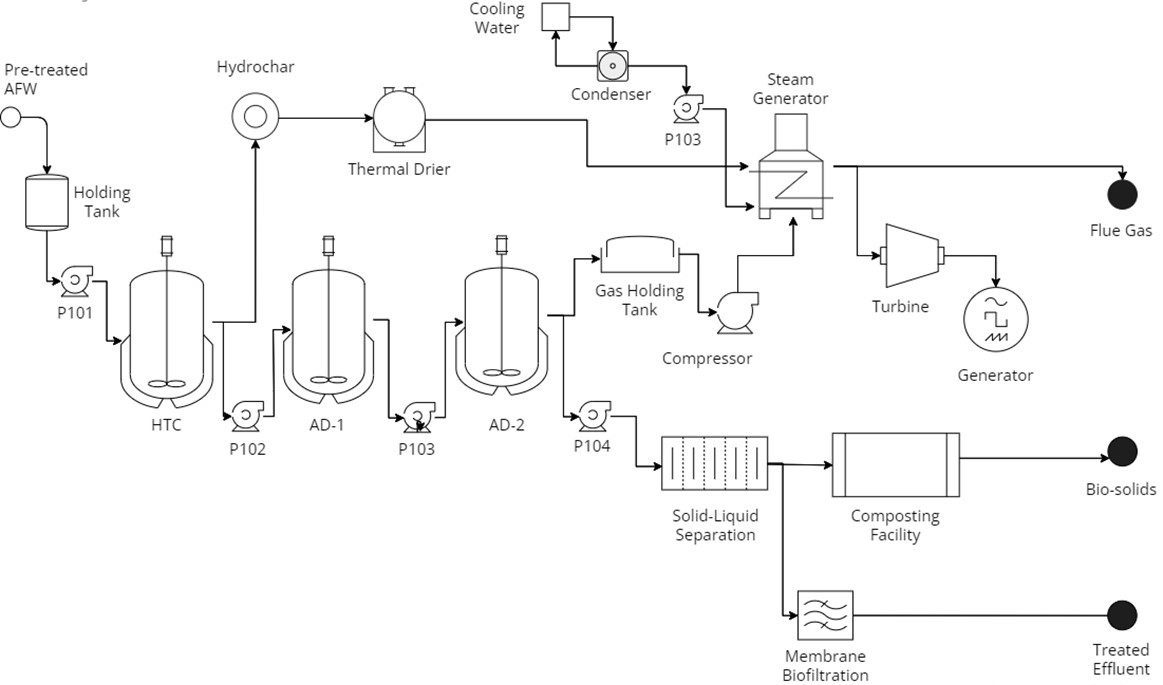


Figure SI-3b Simplified process flow model for S3\_HTC&AD scenario.

**SI-4** **Product conversion reactions with stoichiometric equations, fractional conversion, and kinetic parameters**

Table A: Stoichiometric reactions for modelling hydrolysis in AD reactor 1 (S2\_AD/S3\_HTC & AD)

| No. | Compound | Reactant | Hydrolysis reaction | Fractional Conversion[[1]](#footnote-1) | Fractional Conversion[[2]](#footnote-2) |
| --- | --- | --- | --- | --- | --- |
| 1 | Starch | Maltrose | C6H12O6 + 2 H2O → C2H4O2 + C6H6O3+ 2 H2O | 0.6 ± 0.2 | 0.8 |
| 2 | Cellulose | Levoglucosan | (C6H10O5)n + H2O → C6H12O6 | 0.4 ± 0.1 | 0.3 |
| 3\* | Cellulose | Levoglucosan | C6H12O6 + H2O → 2 C2H6O + 2 CO2 | 0.4 ± 0.1 | 0.3 |
| 4\* | Hemicellulose | Glutaric acid | C5H8O4 + H2O → 2.5 C2H4O2 | 0.5 ± 0.2 | 0.6 |
| 5 | Hemicellulose | Glutaric acid | C5H8O4 + H2O → C5H10O5 | 0.6 ± 0.0 | 0.6 |
| 6 | Xylose | D-Xylose | C5H10O5 → C5H4O2 + 3 H2O | 0.6 ± 0.0 | 0.6 |
| 7\* | Ethanol | Ethanol | 2C2H6O + CO2 → 2 C2H4O2 + CH4 | 0.6 ± 0.1 | 0.5 |
| 8 | Triolein | Triolein | C57H104O6 + 3 H2O → C3H8O3 + 3 C18H34O2 | 0.5 ± 0.2 | 0.7 |
| 9 | Tripalmitin | Tripalmitin | C51H98O6 + 3 H2O → C3H8O3 + 3 C16H34O | 0.5 ± 0.3 | 0.8 |
| 10 | Soluble Protein | - | C13H25O7N3S + 6 H2O → 6.5 CO2 + 6.5 CH4 + 3 H3N + H2S | 0.5 ± 0.2 | 0.9 |
| 11 | Insoluble Protein | Collagen | C4.26H8.56N1.31O2.39S0.02 + 0.08 H2O → 0.1047 C3H7NO2 + 0.0751 C6H14N4O2 + 0.066 C4H8N2O3 + 0.1054 C5H9NO4+ 0.2168 C2H5NO2 + 0.012 C6H9N3O2 + 0.0564 C5H9NO3 + 0.0156 C6H13NO2 + 0.0293 C6H13NO2 + 0.0336 C6H14N2O2+ 0.0224 C5H11NO2S + 0.0301 C9H11NO2 + 0.1346 C5H9NO2 + 0.0342 C3H7NO3+ 0.0282 C4H9NO3 + 0.0131 C9H11NO3 + 0.0225 C5H11NO2 | 0.6 ± 0.1 | 0.7 |
| 12\* | Cholesterol | Palmito-linolein | C37H68O5 + 4.3 H2O → 2.2 C3H8O3 + 0.9 C16H34O + 0.9 C18H32O2 | - | 0.9 |

\*Reactions 1-12 defined for S2\_AD; Reactions 3,4,7,10, 12 only are defined for S3\_HTC & AD

Table B: Stoichiometric reactions and kinetic parameters for modelling HTC reactor (n =1)

| **No.** | **Compound** | **Reactant** | **Hydrolysis Reaction** | **Pre-exponential Factor** | **Activation EnergykJ/kmol** |
| --- | --- | --- | --- | --- | --- |
| Carbohydrate Degradation | | | | | |
| 1 | Starch | Maltrose | C6H12O6 → 5C2H4O2 + C6H6O3+ 2 H2O | 1.11 x 1011 | 147.9 |
| 2 | Cellulose | Levoglucosan | (C6H10O5)n + H2O → C6H12O6 | 5.34 x 109 | 105.1 |
| 3 | Hemicellulose | Glutaric acid | C5H8O4 + H2O → C5H10O5 | 5.42 x 104 | 62.7 |
| 4 | Xylose | D-Xylose | C5H10O5 → 0.075C6H10O7 + 0.3C2H4O2 + 0.75C5H4O2 + 0.2CO2 + 0.55H2 +1.975H2O | 1.19 x 1015 | 146.5 |
| 5 | Glucose | Dextrose | C6H12O6 → C6H6O3 + 3H2O | 5.06 x 109 | 108.0 |
| 6 | 5-HMF | 5-HMF | C6H6O3 + 2H2O → CH2O2 + C5H8O3 | 2.62 x 106 | 89.3 |
| Protein Degradation | | | | | |
| 7 | Protein\* | Collagen | C4.26H8.56N1.31O2.39S0.02 + 0.08 H2O → 0.1047 C3H7NO2 + 0.0751 C6H14N4O2 + 0.066 C4H8N2O3 + 0.1054 C5H9NO4+ 0.2168 C2H5NO2 + 0.012 C6H9N3O2 + 0.0564 C5H9NO3 + 0.0156 C6H13NO2 + 0.0293 C6H13NO2 + 0.0336 C6H14N2O2+ 0.0224 C5H11NO2S + 0.0301 C9H11NO2 + 0.1346 C5H9NO2 + 0.0342 C3H7NO3+ 0.0282 C4H9NO3 + 0.0131 C9H11NO3 + 0.0225 C5H11NO2 | 1.90 x 1020 | 236.5 |
| 8 | Triolein | Triolein | C57H104O6 + 3 H2O → C3H8O3 + 3 C18H34O2 | 1.40 x 1011 | 74 |
| 9 | Tripalmitin | Tripalmitin | C51H98O6 + 3 H2O → C3H8O3 + 3 C16H34O |
| 10 | Cholesterol | Palmito-linolein | C37H68O5 + 4.3 H2O → 2.2 C3H8O3 + 0.9 C16H34O + 0.9 C18H32O2 |

\*Amino acids in Reaction 7 further break down into degradation products using data stoichiometric equations in Table C and kinetic parameters for reaction 7

Table C: Stoichiometric reactions and kinetic parameters for modelling AD reactor 2 (S2\_AD/S3\_HTC & AD)\*

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  | Reactants | | | | Products | | | | | | | | | | | | | | |
|  |  |  | H2O | NH3 | CO2 | H2 | C5H7NO2 | C2H4O2 | NH3 | CO2 | H2 | CH4 | C3H6O2 | C4H8O2 | C5H10O2 | H2O | C2H4O | CH3NO | CH4S | C6H6 | C6H6O |
|  |  | | | | | | | | | | | | | | | | | - | - | - | - |
| Amino acid reactions1 | Alanine | - | - | - | - | - | - | 1 | 1 | 1 | 2 | - | - | - | - | - |  | - | - | - | - |
| Arginine | - | - | - | - | - | - | 2 | 4 | 2 | 3 | - | - | - | - | - |  | - | - | - | - |
| Asparagine | - | - | - | - | - | - | - | 2 | 2 | 1 | - | - | - | - | - | 2 | - | - | - | - |
| Glutamic acid | - | - | - | - | - | - | 2 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - |
| Glycine | C2H5NO2 | - | - | - | - | - | 0.5 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - |
| Histidine | C6H8N3O2 | - | - | - | - | - | 2 | 2 | 1 | 1 | - | - | - | - | - | - | 1 | - | - | - |
| Hydroproline | C5H9NO2 | - | - | - | - | - | 1 | 1 | 2 | 2 | 1 | - | - | - | - | - | - | - | - | - |
| Isoleucine | C6H13NO2 | - | - | - | - | - | - | 1 | 1 | 1 | - | - | - | 1 | - | - | - | - | - | - |
| Leucine | C6H13NO2 | - | - | - | - | - | - | 1 | 1 | 1 | - | - | - | 1 | - | - | - | - | - | - |
| Lysine | C6H14N2O2 | - | - | - | - | - | 1 | 2 | - | - | - | - | 1 | - | - | - | - | - | - | - |
| Methionine | C5H11NO2S | 2 | - | - | - | - | - | 1 | 1 | 1 | - | 1 | - | 1 | - | - | - | 1 | - | - |
| Phenylalanine | C9H11NO2 | 2 | - | - | - | - | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | 1 | - |
| Proline | C5H9NO2 | 4 | - | - | - | - | 2 | - | - | 3 | - | 1 | - | 1 | - | - | - | - | - | - |
| Serine | C3H7NO3 | 1 | - | - | - | - | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | - |
| Threonine | C4H9NO3 | 1 | - | - | - | - | 1 | 1 | 1 | 1 | - | 1 | - | - | - | - | - | - | - | - |
| Tyrosine | C9H11NO3 | 2 | - | - | - | - | 1 | 1 | 1 | 1 | - | - | - | - | - | - | - | - | - | 1 |
| Valine | C5H11NO2 | 2 | - | - | - | - | - | 1 | 1 | 1 | - | - | 1 | - | - | - | - | - | - | - |
| Acidogenic reactions | Dextrose2 | C6H12O6 | - | 0.1115 | - | - | 0.1115 | 0.744 | - | 0.6909 | - | - | 0.5000 | 0.4409 | - | 1.0254 | - | - | - | - | - |
| Glycerol3 | C3H8O3 | - | 0.4071 | 0.0291 | 0.0005 | 0.04071 | - | - | - | - | - | 0.9419 | - | - | 1.0931 | - | - | - | - | - |
| Acetogenic reactions | Oleic acid4 | C18H34O2 | 15.2400 | 0.1701 | 0.2501 |  | 0.1701 | 8.6998 | - | - | 14.4998 | - | - | - | - | - | - | - | - | - | - |
| Propionic acid5 | C3H6O2 | 0.3143 | 0.0620 | - | - | 0.0620 | 0.9345 | - | 0.1607 | 0.0006 | 0.6604 | - | - | - | - | - | - | - | - | - |
| Isobutyric acid6 | C4H8O2 | 0.8038 | 0.0653 | 0.5543 | 0.0006 | 0.0653 | 1.8909 | - | - |  | 0.4460 | - | - | - | - | - | - | - | - | - |
| Isovaleric acid7 | C5H10O2 | 0.8044 | 0.0653 | 0.5543 |  | 0.0653 | 0.8912 | - | - | 0.0006 | 0.4454 | 1 | - | - | - | - | - | - | - | - |
| LCFA-degrading acetogens | Linoleic acid8 | C18H32O2 | 15.2396 | 0.1701 | 0.2501 | - | 0.1701 | 8.6998 | - | - | 13.4998 | - | - | - | - | - | - | - | - | - | - |
| Palmitic acid9 | C16H34O2 | 11.2396 | 0.1701 | 2.2501 | - | 0.1701 | 8.6998 | - | - | 9.4998 | - | - | - | - | - | - | - | - | - | - |
| Methanog-enic reactions | Hydrogen10 | H2 | - | - | 2 | 4 | - | 1 | - | - | - | - | - | - | - | 2 | - | - | - | - | - |
| Acetic acid11 | C2H4O2 | - | 0.022 | - | - | - | 0.022 | - | 0.9450 | - | 0.9450 | - | - | - | 0.066 | - | - | - | - | - |

\*Pre-exponential Factor – 1.4 x 1011; Activation Energy – 74 kJ kmol-1

Table D: Stoichiometric reactions for modelling hydrochar formation in HTC reactions (S3\_HTC&AD)

| No. | Hydrolysis reaction |
| --- | --- |
| 1 | 3 C5H8O3 + 13.5749 H2O --> HYDROCHAR + 22.6979 H2 + 10.2018 CO2 |
| 2 | 2 C5H4O2 + 8.5749 H2O --> HYDROCHAR + 10.2018 CO2 + 9.69787 H2 + 5.2018 CO2 |
| 3 | 2 + 60.5749 H2O --> HYDROCHAR + 91.6979 H2 + 31.2018 CO2 |
| 4 | C6H6O3 + 1.5749 H2O --> HYDROCHAR + 1.6979 H2 + 1.202 CO2 |
| 5 | 2 C3H6O2 + 0.5749 H2O --> HYDROCHAR + 3.6979 H2 + 1.202 CO2 |
| 6 | 4 C2H4O2 + 0.5749 H2O --> HYDROCHAR + 5.6979 H2 + 3.202 CO2 |
| 7 | 2 C4H8O2 + 4.5749 H2O --> HYDROCHAR + 9.6979 H2 + 3.202 CO2 |
| 8 | 3 C3H8O3 + 1.5749 H2O --> HYDROCHAR + 10.6979 H2 + 4.202 CO2 |
| 9 | 2 C5H10O2 + 8.5749 H2O --> HYDROCHAR + 15.6979 H2 + 5.202 CO2 |
| 10 | 2 C6H10O7 + 2.5749 H2O --> HYDROCHAR + 9.6979 H2 + 7.202 CO2 |
| 11 | 2 C18H32O2 + 60.5749 H2O --> HYDROCHAR + 31.202 CO2 + 89.6979 H2 |
| 12 | 5 CH2O2 + 0.377 H2O --> HYDROCHAR + 0.2018 CO2 + 4.0511 O2 |

**SI-5 Transfer coefficients mobilised for modelling agri-food market waste MFA for all scenarios**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | | **Transfer coefficients of “goods” (i.e., bulk wastes, products, residues, or emissions) and “substances” (i.e., heavy metals)** | | | | | | | |
| **Processes** | **Description of flows** | **As ‘goods’** | **As ‘substances’** | | | | | | |
| **Zn** | **Cu** | **Cr** | **Ni** | **Pb** | **Cd** | **Hg** |
| **Separation** | As organic fractions1 (OFRAC) | 0.92 ± 0.03 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| As mixed inorganic\* residues | 0.08 ± 0.03 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| **Sorting & selection of easily digestible AD substrates** | Easily digested2 OFRAC | 0.75 ± 0.10 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| Non-easily digested OFRAC\* | 0.25 ± 0.10 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| **Size reduction and homogenisation** | Homogenised3  OFRAC | 0.95 ± 0.32 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| Process  losses3 | 0.05 ± 0.32 | Same as the transfer coefficient used for ‘goods’ | | | | | | |
| **AD treatment** | As biogas  production3 | 0.12 ± 0.11 | - | - | - | 0.12 ± 0.96 | - | - | 0.12 ± 0.96 |
| As digestate  (slurry)\* | 0.86 ± 0.11 | 1.00 ± 0.00 | 1.00 ± 0.00 | 1.00 ± 0.00 | 0.86 ± 0.96 | 1.00 ± 0.00 | 1.00 ± 0.00 | 0.86 ± 0.96 |
| As emission to air  (losses)3 | 0.02 ± 0.11 | - | - | - | 0.02 ± 0.96 | - | - | 0.02 ± 0.96 |
| **HTC treatment4,5** | As hydrochar  (Solid fraction) | 0.70 ± 0.10 | 0.32 ± 0.10 | 0.61 ± 0.10 | 0.45 ± 0.10 | 0.22 ± 0.10 | 0.94 ± 0.10 | 0.24 ± 0.10 | 0.95 ± 0.10 |
| As process water to AD conversion | 0.25 ± 0.10 | 0.68 ± 0.10 | 0.39 ± 0.10 | 0.55 ± 0.10 | 0.78 ± 0.10 | 0.06 ± 0.10 | 0.76 ± 0.10 | 0.05 ± 0.10 |
| As gaseous emission (losses) to air | 0.05 ± 0.10 | Heavy metal concentration is negligible. | | | | | | |
| **Solid-liquid separation (via centrifugation),6,7** | Solid fraction to aerobic composting | 0.125 ± 0.025 | 0.97 ± 0.013 | 0.97 ± 0.004 | 0.88 ± 0.04 | 0.49 ± 0.05 | 0.97 ± 0.01 | 0.98 ± 0.014 | 0.95 ± 0.10 |
| Liquid effluent fraction for treatment | 0.875 ± 0.025 | 0.03 ± 0.013 | 0.03 ± 0.004 | 0.12 ± 0.04 | 0.51 ± 0.05 | 0.03 ± 0.01 | 0.02 ± 0.014 | 0.05 ± 0.10 |
| **Effluent treatment by MBR 3,8,9** | As permeate (treated effluent) | 0.5 ± 0.10 | 0.13 ± 0.10 | 0.02 ± 0.10 | 0.09 ± 0.10 | 0.18 ± 0.10 | 0.01 ± 0.10 | 0.04 ± 0.10 | 0.03 ± 0.10 |
| Concentrate (process rejects) | 0.5 ± 0.10 | 0.87 ± 0.10 | 0.98 ± 0.10 | 0.91 ± 0.10 | 0.82 ± 0.10 | 0.99 ± 0.10 | 0.96 ± 0.10 | 0.97 ± 0.10 |
| **Aerobic composting** | As compost3 | 0.36 ± 0.11 | 0.75 ± 0.32 | 0.67 ± 0.32 | 0.96 ± 0.32 | 0.36 ± 0.96 | 0.59 ± 0.32 | 0.50 ± 0.32 | 0.86 ± 0.32 |
| As emission to air  (losses)3 | 0.52 ± 0.11 | - | - | - | 0.52 ± 0.96 | - | - | - |
| Compost residues to landfill\* | 0.12 ± 0.11 | 0.25 ± 0.32 | 0.33 ± 0.32 | 0.04 ± 0.32 | 0.12 ± 0.96 | 0.41 ± 0.32 | 0.50 ± 0.32 | 0.14 ± 0.32 |

**Notes**

For all transfer coefficients collated or estimated without a stated standard error, a conservative 10% uncertainty was assumed.

\* Estimated by difference, i.e., 1 – (transfer coefficients of all other flows)

1 Based on the average organic fractions from the three markets. Estimated from Byrne et, 2015 [***Source****: Byrne, A., Gold, M., Turyasiima, D., Getkate, W., Niwagaba, C., Babu, M., Maiteki, J., Orwiny, M., Strande, L., 2015. Sludge to Energy Enterprises in Kampala (SEEK) Project. Suitable biowastes for energy recovery. [Online]* [*http://www.eawag.ch/fileadmin/Domain1/Abteilungen/sandec/schwerpunkte/ewm/SEEK/pdfs/seek\_suitable\_waste\_streams.pdf*](http://www.eawag.ch/fileadmin/Domain1/Abteilungen/sandec/schwerpunkte/ewm/SEEK/pdfs/seek_suitable_waste_streams.pdf).

2 Organic fractions of fruit and vegetables from open urban markets in Tunisia. [***Source****: Bouallagui, H., Touhami, Y., Ben Cheikh, R., Hamdi, M., 2005. Bioreactor performance in anaerobic digestion of fruit and vegetable wastes, Process Biochemistry, 40 (3–4), 989-995,* [*https://doi.org/10.1016/j.procbio.2004.03.007*](https://doi.org/10.1016/j.procbio.2004.03.007)*]*

3 Transfer coefficients for ‘goods’ and ‘substances’ extracted from Allesch, A. and Brunner, P.H., 2017. [***Source****: Allesch, A. and Brunner, P.H., 2017. Material flow analysis as a tool to improve waste management systems: The case of Austria. Environ. Sci. Technol. 51, 540 – 551*]. The transfer coefficients for losses or products (e.g., compost and biogas) were first collated, and the difference was assumed as the transfer coefficients by-products/residuals.

4 Bulk ‘goods’ transfer coefficients of HTC products were informed by several studies, including Libra et al, 2011 [***Source****: Libra, J.A., Ro, K.S., Kammann, C., Funke, A., Berge, N.D., Neubauer, Y., Titirici, M.M., Fühner, C., Bens, O., Kern, J., Emmerich, K.H., 2011. Hydrothermal carbonisation of biomass residuals: a comparative review of the chemistry, processes and applications of wet and dry pyrolysis. Biofuels 2, 71–106. doi:10.4155/bfs.10.81*] and Hoekman et al, 2013 [***Source***: *Hoekman, S.K., Broch, A., Robbins, C., Zielinska, B., Felix, L., 2013. Hydrothermal carbonisation (HTC) of selected woody and herbaceous biomass feedstocks. Biomass Conv. Bioref. 3, 113–126.* [*https://doi.org/10.1007/s13399-012-0066-y*](https://doi.org/10.1007/s13399-012-0066-y)*].*

5 The transfer coefficients of heavy metals in HTC products were estimated from HM concentration in one kg of raw and hydrochar recovered from corn stover [***Source:*** *Reza, M.T, Lynam, J.G., Uddin, M.H, Coronella, C.J., 2013. Hydrothermal carbonisation: Fate of inorganics. Biomass and Bioenergy 49: 86–94*]. Guided by this literature, a conservative 95% of total concentration retained in hydrochar was assumed for Hg. A conservative 10% uncertainty was assumed for all transfer coefficients.

6 Bulk ‘goods’ transfer coefficients informed by the percentage of a full-scale industrial solid-liquid-separation system deployed for digestates using decanter centrifugation. [***Source****: Karakashev, D., Schmidt, J.E., Angelidaki, I., 2008. Innovative process scheme for removal of organic matter, phosphorus and nitrogen from pig manure. Water Res. 42, 4083–4090.* [*https://doi.org/10.1016/J.WATRES.2008.06.021*](https://doi.org/10.1016/J.WATRES.2008.06.021)].

7 The transfer coefficients of heavy metals data were aggregated from the element concentrations in centrifuged digestates samples in Valeur, 2011 [***Source***: *Valeur, I., 2011. Speciation of heavy metals and nutrient elements in digestates. MSc Thesis – Norwegian Uni. of Life Science*] and validated against Zhu et al. 2014 [***Source***: *Zhu, N.M., Li, Q., Guo, X.J., Zhang, H., Deng, Y., 2014. Sequential extraction of anaerobic digestate sludge to determine the partitioning of heavy metals. Ecotoxicology Environmental Safety. 102, 18–24*]. The percentage difference for most heavy metals in the liquid effluent was less than 10%.

8 Bulk ‘goods’ transfer coefficients at the effluent treatment stage was extracted from Bolzonella et al. 2018 [***Source:*** *Bolzonella, D., Fatone, F., Gottardo, M., Frison, N., 2018. Nutrients recovery from anaerobic digestate of agro-waste: Techno-economic assessment of full-scale applications. J. Environ. Manage. 216, 111–119.* [*https://doi.org/10.1016/J.JENVMAN.2017.08.026*](https://doi.org/10.1016/J.JENVMAN.2017.08.026)*),* which reported 50% of original w/w of digestate treated via membrane technology (with 70 – 80% recovery efficiency) recovery as clean water.

9 The transfer coefficients of heavy metals at the effluent treatment stage were estimated from large scale UF plant under real-life operational conditions from Arévalo et al, 2013 [***Source***: *Arévalo J, Ruiz LM, Pérez J, Moreno B, Gómez MÁ, 2013. The removal performance of heavy metals in MBR systems and their influence on water reuse. Water Sci Technol.;67(4):894-900. Doi: 10.2166/wst.2012.620*]. A conservative 10% uncertainty was assumed for all transfer coefficients. These were validated against Camilleri-Rumbau et al, 2019. [***Source:*** *Camilleri-Rumbau M.S.; Popovic, O.; Briceno, K.; Errico, M.; Søtoft, L.F.; Christensen, K.V.; Norddahl, B. Ultrafiltration of separated digestate by tubular membranes: Influence of feed pre-treatment on hydraulic performance and heavy metal removal. J. Environ. Manag. 2019, 250, 109404*]. Guided by this literature and Ref in note 3, a conservative 97% removal efficiency was assumed for Hg.

**SI-6** **Substance flow balances (t yr-1) aggregated for all agri-food markets for S2\_AD**

**Diagram

Description automatically generated**

Figure SI-6A SFA for Cu

**Diagram

Description automatically generated**

Figure SI-6B SFA for Pb

**Diagram

Description automatically generated**

Figure SI-6C SFA for Cr

**Diagram

Description automatically generated**

Figure SI-6D SFA for Ni

**Diagram

Description automatically generated**

Figure SI-6E SFA for Cd

**Diagram

Description automatically generated**

Figure SI-6F SFA for Hg

**Diagram

Description automatically generated**

Figure SI-6G SFA for Zn

**SI-7** **Substance flow balances (t yr-1) aggregated for all agri-food markets for S3\_HTC&AD**

**Diagram

Description automatically generated**

Figure SI-7A SFA for Cu

**Diagram

Description automatically generated**

Figure SI-7B SFA for Pb

**Diagram

Description automatically generated**

Figure SI-7C SFA for Cr

**Diagram

Description automatically generated**

Figure SI-7D SFA for Ni

**Diagram

Description automatically generated**

Figure SI-7E SFA for Cd

**Diagram

Description automatically generated**

Figure SI-7F SFA for Hg

**Diagram

Description automatically generated**

Figure SI-7G SFA for Zn

**SI-8** **Sensitivity Analysis Input Data for S2\_AD & S3\_HTC&AD**

|  |  |  |
| --- | --- | --- |
|  | S2\_AD & S3\_HTC&AD | |
| Scenarios | Lower Boundary | Upper Boundary |
| 1. Cumulative pre-processing loss of AFW (%) | 31.0 | 37.9 |
| 1. Percentage of effluent treated via MBR (%) | 45.0 | 55.0 |
| 1. Percentage of solid-liquid separation (%) | 11.3 | 13.8 |
| 1. Biogas yield as a proportion of biodegradable carbon (%) | 63 | 77 |

**Supplementary Information Reference**

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1. Rajendran, K et [7] [↑](#footnote-ref-1)
2. Values used in this study [↑](#footnote-ref-2)