

Supplementary material

Aspen Plus® process simulation model of the biomass ash-based treatment of anaerobic digestate for production of fertilizer and upgradation of biogas

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Table S1. Mass balance of the nutrients monitored in the Aspen Plus® simulations. (1/3)

| Stream | Parameter | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 | Case 6 | Case 7 |
|------------------|-----------------------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Biogas | Carbon Dioxide/(vol.%) | 3.43E+01 | 5.77E+01 | 5.82E+01 | 5.92E+01 | 5.65E+01 | 1.42E+01 | 4.77E-05 |
| | Ammonia/(vol.%) | 4.61E-05 | 4.61E-04 | 1.00E-01 | 6.56E-02 | 1.18E-02 | 1.77E+01 | 7.49E+00 |
| | Methane/(vol.%) | 4.88E+01 | 2.78E+01 | 2.69E+01 | 2.60E+01 | 2.86E+01 | 5.48E+01 | 7.83E+01 |
| Digestate | pH | 7.41 | 7.40 | 4.10 | 3.24 | 9.26 | 12.34 | 13.24 |
| Nitrogen | Organic flow/(mol/hr) | 1.01E-03 | 1.31E-03 | 9.86E-04 | 9.80E-04 | 9.97E-04 | 9.51E-04 | 2.25E-03 |
| | Inorganic flow/(mol/hr) | 3.50E-05 | 1.91E-03 | 4.85E-03 | 4.65E-03 | 5.09E-04 | 2.16E-02 | 9.70E-03 |
| | Organic fraction/(mol.%) | 1.90E-03 | 2.08E-03 | 1.64E-03 | 1.63E-03 | 1.66E-03 | 1.44E-03 | 3.39E-03 |
| | Inorganic fraction/(mol.%) | 6.60E-05 | 3.05E-03 | 8.09E-03 | 7.75E-03 | 8.49E-04 | 3.26E-02 | 1.47E-02 |
| | Organic N/(g/l) | 9.53E-02 | 6.69E-02 | 5.59E-02 | 5.56E-02 | 5.76E-02 | 5.39E-02 | 9.70E-02 |
| | Inorganic N/(g/l) | 3.32E-03 | 9.80E-02 | 2.75E-01 | 2.64E-01 | 2.94E-02 | 1.22E+00 | 4.19E-01 |
| | WS flow/(mol/hr) | 1.04E-03 | 1.30E-03 | 1.12E-03 | 1.07E-03 | 9.96E-04 | 9.44E-04 | 2.25E-03 |
| | WI flow/(mol/hr) | 5.66E-06 | 1.16E-03 | 4.03E-04 | 1.31E-04 | 5.10E-04 | 2.16E-02 | 9.70E-03 |
| | WS fraction/(mol.%) | 1.95E-01 | 2.08E-01 | 1.86E-01 | 1.78E-01 | 1.66E-01 | 1.43E-01 | 3.39E-01 |
| | WI fraction/(mol.%) | 1.07E-03 | 1.85E-01 | 6.73E-02 | 2.18E-02 | 8.51E-02 | 3.26E+00 | 1.47E+00 |
| | WS N/(mol/l) | 9.81E-02 | 6.68E-02 | 6.33E-02 | 6.04E-02 | 5.75E-02 | 5.35E-02 | 9.70E-02 |
| | WI N/(mol/l) | 5.36E-04 | 5.93E-02 | 2.29E-02 | 7.41E-03 | 2.95E-02 | 1.22E+00 | 4.19E-01 |

Table S2. Mass balance of the nutrients monitored in the Aspen Plus® simulations. (2/3)

| Element | Parameter | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 | Case 6 | Case 7 |
|--------------------|----------------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Phosphorous | WS flow/(mol/hr) | 4.72E-04 | 1.90E-03 | 1.94E-03 | 1.24E-03 | 1.60E-03 | 2.42E-03 | 1.92E-03 |
| | WI flow/(mol/hr) | 1.04E-05 | 2.35E-13 | 0.00E+00 | 0.00E+00 | 6.91E-05 | 0.00E+00 | 0.00E+00 |
| | WS fraction/(mol.%) | 8.90E-03 | 3.03E-01 | 3.24E-01 | 2.07E-01 | 2.67E-01 | 3.65E-01 | 2.90E-01 |
| | WI fraction/(mol.%) | 1.96E-03 | 3.75E-11 | 0.00E+00 | 0.00E+00 | 1.15E-02 | 0.00E+00 | 0.00E+00 |
| | WS P/(mol/l) | 4.47E-03 | 9.74E-02 | 1.10E-01 | 7.03E-02 | 9.25E-02 | 1.37E-01 | 8.29E-02 |
| | WI P/(mol/l) | 9.85E-04 | 1.20E-11 | 0.00E+00 | 0.00E+00 | 3.99E-03 | 0.00E+00 | 0.00E+00 |
| Potassium | WS flow/(mol/hr) | 8.81E-04 | 1.09E-02 | 3.52E-03 | 3.63E-03 | 4.20E-03 | 3.04E-03 | 1.93E-03 |
| | WI flow/(mol/hr) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 8.67E-04 |
| | WS fraction/(%) | 1.66E-01 | 1.74E+00 | 5.88E-01 | 6.06E-01 | 7.01E-01 | 4.59E-01 | 2.91E-01 |
| | WI fraction/(%) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 1.31E-01 |
| | WS K/(mol/l) | 8.35E-02 | 5.59E-01 | 2.00E-01 | 2.06E-01 | 2.43E-01 | 1.72E-01 | 8.33E-02 |
| | WI K/(mol/l) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 3.74E-02 |
| Carbon | WS flow/(mol/hr) | 2.77E-03 | 4.97E-03 | 3.49E-03 | 3.43E-03 | 3.54E-03 | 6.78E-03 | 7.89E-03 |
| | WI flow/(mol/hr) | 3.42E-04 | 8.24E-04 | 3.27E-04 | 3.26E-04 | 3.26E-04 | 3.78E-04 | 6.19E-04 |
| | WS fraction/(mol.%) | 5.22E-01 | 7.92E-01 | 5.83E-01 | 5.71E-01 | 5.90E-01 | 1.02E+00 | 1.19E+00 |
| | WI fraction/(mol.%) | 6.45E-02 | 1.31E-01 | 5.45E-02 | 5.44E-02 | 5.44E-02 | 5.72E-02 | 9.35E-02 |
| | WS C/(mol/l) | 2.62E-01 | 2.54E-01 | 1.98E-01 | 1.94E-01 | 2.04E-01 | 3.84E-01 | 3.41E-01 |
| | WI C/(mol/l) | 3.24E-02 | 4.22E-02 | 1.85E-02 | 1.85E-02 | 1.89E-02 | 2.15E-02 | 2.67E-02 |

Table S3. Mass balance of the nutrients tracked in the Aspen Plus® simulations. (3/3)

| Element | Parameter | Case 1 | Case 2 | Case 3 | Case 4 | Case 5 | Case 6 | Case 7 |
|------------------|----------------------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
| Magnesium | WS flow/(mol/hr) | 2.44E-04 | 2.77E-03 | 3.16E-03 | 2.99E-03 | 3.25E-03 | 8.92E-03 | 9.79E-03 |
| | WI flow/(mol/hr) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| | WS fraction/(mol.%) | 4.60E-02 | 4.41E-01 | 5.26E-01 | 4.98E-01 | 5.43E-01 | 1.35E+00 | 1.48E+00 |
| | WI fraction/(mol.%) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| | WS Mg/(mol/l) | 2.31E-02 | 1.42E-01 | 1.79E-01 | 1.69E-01 | 1.88E-01 | 5.06E-01 | 4.23E-01 |
| | WI Mg/(mol/l) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| Calcium | WS flow/(mol/hr) | 1.76E-04 | 6.66E-03 | 3.19E-03 | 3.53E-03 | 4.00E-03 | 8.28E-03 | 8.11E-03 |
| | WI flow/(mol/hr) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| | WS fraction/(mol.%) | 3.32E-02 | 1.06E+00 | 5.33E-01 | 5.89E-01 | 6.67E-01 | 1.25E+00 | 1.22E+00 |
| | WI fraction/(mol.%) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| | WS Ca/(mol/l) | 1.67E-02 | 3.41E-01 | 1.81E-01 | 2.00E-01 | 2.31E-01 | 4.70E-01 | 3.50E-01 |
| | WI Ca/(mol/l) | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| Sulphur | WS flow/(mol/hr) | 1.17E-05 | 1.32E-03 | 5.24E-06 | 6.80E-04 | 2.53E-06 | 3.20E-03 | 3.60E-03 |
| | WI flow/(mol/hr) | 6.57E-07 | 2.89E-06 | 2.08E-06 | 1.98E-06 | 1.95E-06 | 1.00E-05 | 1.01E-05 |
| | WS fraction/(mol.%) | 2.21E-03 | 2.11E-01 | 8.74E-04 | 1.13E-01 | 4.22E-04 | 4.83E-01 | 5.44E-01 |
| | WI fraction/(mol.%) | 1.24E-04 | 4.61E-04 | 3.47E-04 | 3.31E-04 | 3.25E-04 | 1.51E-03 | 1.53E-03 |
| | WS S/(mol/l) | 1.11E-03 | 6.76E-02 | 2.97E-04 | 3.86E-02 | 1.46E-04 | 1.81E-01 | 1.55E-01 |
| | WI S/(mol/l) | 6.23E-05 | 1.48E-04 | 1.18E-04 | 1.13E-04 | 1.13E-04 | 5.69E-04 | 4.36E-04 |

Table S4. List of the components in the PSM of Rajendran et al. [11]. (1/3)

| Component ID | Type | Component name | Alias |
|---|--------------|------------------------------|---|
| WATER | Conventional | WATER | H ₂ O |
| GLYCEROL | Conventional | GLYCEROL | C ₃ H ₈ O ₃ |
| OLEIC-AC | Conventional | OLEIC-ACID | C ₁₈ H ₃₄ O ₂ |
| DEXTROSE | Conventional | DEXTROSE | C ₆ H ₁₂ O ₆ |
| ACETI-AC | Conventional | ACETIC-ACID | C ₂ H ₄ O ₂ |
| PROPI-01 | Conventional | PROPIONIC-ACID | C ₃ H ₆ O ₂ |
| ISOBU-01 | Conventional | ISOBUTYRIC-ACID | C ₄ H ₈ O ₂ |
| ISOVA-01 | Conventional | ISOVALERIC-ACID | C ₅ H ₁₀ O ₂ |
| H ⁺ | Conventional | H ⁺ | H ⁺ |
| OH ⁻ | Conventional | OH ⁻ | OH ⁻ |
| NH ₃ | Conventional | AMMONIA | NH ₃ |
| NH ₄ ⁺ | Conventional | NH ₄ ⁺ | NH ₄ ⁺ |
| CO ₂ | Conventional | CARBON-DIOXIDE | CO ₂ |
| C ₅ H ₇ NO ₂ | Conventional | ETHYL-CYANOACETATE | C ₅ H ₇ NO ₂ |
| ARGININE | Conventional | ARGININE | C ₆ H ₁₄ N ₄ O ₂ |
| HISTIDIN | Conventional | HISTIDINE-E-2 | C ₆ H ₈ N ₃ O ₂ |
| LYSINE | Conventional | LYSINE | C ₆ H ₁₄ N ₂ O ₂ |
| TYROSINE | Conventional | TYROSINE | C ₉ H ₁₁ NO ₃ |
| TRYPTOPH | Conventional | TRYPTOPHAN | C ₁₁ H ₁₂ N ₂ O ₂ |
| PHENYLAL | Conventional | L-PHENYLALANINE | C ₉ H ₁₁ NO ₂ |
| CYSTEINE | Conventional | CYSTEINE-E-2 | C ₃ H ₆ NO ₂ S |
| METHIONI | Conventional | METHIONINE | C ₅ H ₁₁ NO ₂ S |
| THREONIN | Conventional | THREONINE | C ₄ H ₉ NO ₃ |
| SERINE | Conventional | SERINE | C ₃ H ₇ NO ₃ |
| LEUCINE | Conventional | LEUCINE | C ₆ H ₁₃ NO ₂ |
| ISOLEUCI | Conventional | ISOLEUCINE | C ₆ H ₁₃ NO ₂ |

Table S5. List of the components in the PSM of Rajendran et al. [11]. (2/3)

| Component ID | Type | Component name | Alias |
|--------------------------------|--------------|-------------------------------|---|
| VALINE | Conventional | VALINE | C ₅ H ₁₁ NO ₂ |
| GLUTAMIC | Conventional | L-GLUTAMIC-ACID | C ₅ H ₉ NO ₄ |
| ASPARTIC | Conventional | ASPARTIC-ACID | C ₄ H ₇ NO ₄ |
| GLYCINE | Conventional | GLYCINE | C ₂ H ₅ NO ₂ |
| ALANINE | Conventional | ALANINE | C ₃ H ₇ NO ₂ |
| PROLINE | Conventional | PROLINE | C ₅ H ₉ NO ₂ |
| HYDROGEN | Conventional | HYDROGEN | H ₂ |
| METHANE | Conventional | METHANE | CH ₄ |
| INDOLE | Conventional | INDOLE | C ₈ H ₇ N |
| FROMAMID | Conventional | FORMAMIDE | CH ₃ NO |
| H ₂ S | Conventional | HYDROGEN-SULFIDE | H ₂ S |
| CH ₄ S | Conventional | METHYL-MERCAPTAN | CH ₄ S |
| BENZENE | Conventional | BENZENE | C ₆ H ₆ |
| PHENOL | Conventional | PHENOL | C ₆ H ₆ O |
| H ₂ CO ₃ | Conventional | CARBONIC-ACID | H ₂ CO ₃ |
| HCO ₃ ⁻ | Conventional | HCO ₃ ⁻ | HCO ₃ ⁻ |
| CO ₃ ²⁻ | Conventional | CO ₃ ²⁻ | CO ₃ ²⁻ |
| HS ⁻ | Conventional | HS ⁻ | HS ⁻ |
| CELLULOS | Conventional | CELLULOSE | CELLULOSE |
| HEMECELL | Conventional | GLUTARIC-ACID | C ₅ H ₈ O ₄ |
| GLUCOSE | Conventional | DEXTROSE | C ₆ H ₁₂ O ₆ |
| TRIOLEIN | Conventional | TRIOLEIN | C ₅₇ H ₁₀₄ O ₆ |
| TRIPALM | Conventional | TRIPALMITIN | C ₅₁ H ₉₈ O ₆ |
| PALM | Conventional | 1-HEXADECANOL | C ₁₆ H ₃₄ O |
| SN-1--01 | Conventional | SN-1-PALMITO-2-OLEIN | C ₃₇ H ₇₀ O ₅ |
| SN-1--02 | Conventional | SN-1-PALMITO-2-LINOLEIN | C ₃₇ H ₆₈ O ₅ |

Table S6. List of the components in the PSM of Rajendran et al. [11]. (3/3)

| Component ID | Type | Component name | Alias |
|----------------------------------|-----------------|----------------------------------|---|
| XYLOSE | Conventional | D-XYLOSE | C ₅ H ₁₀ O ₅ |
| FURFURAL | Conventional | FURFURAL | C ₅ H ₄ O ₂ |
| LINOLEIC | Conventional | LINOLEIC-ACID | C ₁₈ H ₃₂ O ₂ |
| STARCH | Conventional | CELLULOSE | CELLULOSE |
| ETHANOL | Conventional | ETHANOL | C ₂ H ₆ O |
| PROTEIN | Pseudocomponent | | C ₁₃ H ₂₅ O ₇ N ₃ S |
| KERATIN | Pseudocomponent | | C _{4.39} H ₈ NO _{2.1} |
| ACETATE | Conventional | CH ₃ COO ⁻ | CH ₃ COO ⁻ |
| INERT | Pseudocomponent | | INERT |
| AMMON(S) | Solid | AMMONIUM-CARBAMATE | NH ₂ COONH ₄ |
| NH ₄ HS (S) | Solid | AMMONIUM-HYDROGEN-SULFIDE | NH ₄ HS |
| NH ₄ HCO ₃ | Solid | AMMONIUM-HYDROGEN-CARBONATE | NH ₄ HCO ₃ |
| NH ₂ COO ⁻ | Conventional | CARBAMATE | NH ₂ COO ⁻ |
| S ²⁻ | Conventional | S ²⁻ | S ²⁻ |