# 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 | H2O |
| GLYCEROL | Conventional | GLYCEROL | C3H8O3 |
| OLEIC-AC | Conventional | OLEIC-ACID | C18H34O2 |
| DEXTROSE | Conventional | DEXTROSE | C6H12O6 |
| ACETI-AC | Conventional | ACETIC-ACID | C2H4O2 |
| PROPI-01 | Conventional | PROPIONIC-ACID | C3H6O2 |
| ISOBU-01 | Conventional | ISOBUTYRIC-ACID | C4H8O2 |
| ISOVA-01 | Conventional | ISOVALERIC-ACID | C5H10O2 |
| H+ | Conventional | H+ | H+ |
| OH- | Conventional | OH- | OH- |
| NH3 | Conventional | AMMONIA | NH3 |
| NH4+ | Conventional | NH4+ | NH4+ |
| CO2 | Conventional | CARBON-DIOXIDE | CO2 |
| C5H7NO2 | Conventional | ETHYL-CYANOACETATE | C5H7NO2 |
| ARGININE | Conventional | ARGININE | C6H14N4O2 |
| HISTIDIN | Conventional | HISTIDINE-E-2 | C6H8N3O2 |
| LYSINE | Conventional | LYSINE | C6H14N2O2 |
| TYROSINE | Conventional | TYROSINE | C9H11NO3 |
| TRYPTOPH | Conventional | TRYPTOPHAN | C11H12N2O2 |
| PHENYLAL | Conventional | L-PHENYLALANINE | C9H11NO2 |
| CYSTEINE | Conventional | CYSTEINE-E-2 | C3H6NO2S |
| METHIONI | Conventional | METHIONINE | C5H11NO2S |
| THREONIN | Conventional | THREONINE | C4H9NO3 |
| SERINE | Conventional | SERINE | C3H7NO3 |
| LEUCINE | Conventional | LEUCINE | C6H13NO2 |
| ISOLEUCI | Conventional | ISOLEUCINE | C6H13NO2 |

**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 | C5H11NO2 |
| GLUTAMIC | Conventional | L-GLUTAMIC-ACID | C5H9NO4 |
| ASPARTIC | Conventional | ASPARTIC-ACID | C4H7NO4 |
| GLYCINE | Conventional | GLYCINE | C2H5NO2 |
| ALANINE | Conventional | ALANINE | C3H7NO2 |
| PROLINE | Conventional | PROLINE | C5H9NO2 |
| HYDROGEN | Conventional | HYDROGEN | H2 |
| METHANE | Conventional | METHANE | CH4 |
| INDOLE | Conventional | INDOLE | C8H7N |
| FROMAMID | Conventional | FORMAMIDE | CH3NO |
| H2S | Conventional | HYDROGEN-SULFIDE | H2S |
| CH4S | Conventional | METHYL-MERCAPTAN | CH4S |
| BENZENE | Conventional | BENZENE | C6H6 |
| PHENOL | Conventional | PHENOL | C6H6O |
| H2CO3 | Conventional | CARBONIC-ACID | H2CO3 |
| HCO3- | Conventional | HCO3- | HCO3- |
| CO32- | Conventional | CO32- | CO32- |
| HS- | Conventional | HS- | HS- |
| CELLULOS | Conventional | CELLULOSE | CELLULOSE |
| HEMECELL | Conventional | GLUTARIC-ACID | C5H8O4 |
| GLUCOSE | Conventional | DEXTROSE | C6H12O6 |
| TRIOLEIN | Conventional | TRIOLEIN | C57H104O6 |
| TRIPALM | Conventional | TRIPALMITIN | C51H98O6 |
| PALM | Conventional | 1-HEXADECANOL | C16H34O |
| SN-1--01 | Conventional | SN-1-PALMITO-2-OLEIN | C37H70O5 |
| SN-1--02 | Conventional | SN-1-PALMITO-2-LINOLEIN | C37H68O5 |

**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 | C5H10O5 |
| FURFURAL | Conventional | FURFURAL | C5H4O2 |
| LINOLEIC | Conventional | LINOLEIC-ACID | C18H32O2 |
| STARCH | Conventional | CELLULOSE | CELLULOSE |
| ETHANOL | Conventional | ETHANOL | C2H6O |
| PROTEIN | Pseudocomponent |  | C13H25O7N3S |
| KERATIN | Pseudocomponent |  | C4.39H8NO2.1 |
| ACETATE | Conventional | CH3COO- | CH3COO- |
| INERT | Pseudocomponent |  | INERT |
| AMMON(S) | Solid | AMMONIUM-CARBAMATE | NH2COONH4 |
| NH4HS (S) | Solid | AMMONIUM-HYDROGEN-SULFIDE | NH4HS |
| NH4HCO3 | Solid | AMMONIUM-HYDROGEN-CARBONATE | NH4HCO3 |
| NH2COO- | Conventional | CARBAMATE | NH2COO- |
| S2- | Conventional | S2- | S2- |