**Optimal integrated facility for waste processing**

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All the units involved in the flowsheet are modelled using mass and energy balances, thermodynamic relationships, chemical and vapor-liquid equilibria, and product yield calculations. Therefore, the variables of the equation oriented framework comprise the total mass flows, component mass flows, component mass fractions, temperatures and pressures of the streams in the process network. The components that are tracked in our calculations belong to the set {Wa, CO2, CO, O2, N2, H2S, NH3, CH4, SO2, C, H, O, N, Norg, P, K, S, Rest, Cattle\_slurry, Pig\_slurry, Poultry\_slurry, P2O5, K2O, CaCO3, FeCl3, Antifoam, Fe2SO4\_3, Al2SO4\_3, AlCl3, MgCl2, NaOH, Struvite\_seeds, Mg, Cl, Struvite, KStruvite, MgCl2\_CSTR, NaOH\_CSTR, Mg\_CSTR, Cl\_CSTR, Struvite\_CSTR, KStruvite\_CSTR, FeCl3\_Coag}. In the following subsections we briefly present the main equations used to characterize the operation of the different units. Simpler balances based on removal efficiency or stoichiometry, or the equations that connect two units are omitted and only the conversion, the chemical reactions, and the removal efficiency are presented.

The decision on the technology to use to process the digestate requires the evaluation of the cost. Its estimation uses the factorial method based on the equipment units costs Sinnot (1999). The total physical plant cost involving equipment erection, piping instrumentation, electrical, buildings, utilities, storages, site development, and ancillary buildings is 3.15 times the total equipment cost for processes which uses fluids and solids. On the other hand, the fixed cost, which includes design and engineering, contractor’s fee, and contingency items is determined as 1.4 times the total physical plant cost for fluid and solid processes. In the subsequent cost estimation these parameters are designed as fi for the total physical plant parameter and fj for the fixed cost parameter.

**S.1.-Biogas production**

The anaerobic fermentation of different types of manure generates biogas, methane and carbon dioxide, through a series of reactions such as hydrolysis, acidogenesis, acetogenesis and methanogenesis (Al Seadi et al., 2008). The biogas produced shows a variable composition in methane and CO2 depending on the composition of the manure processed and the operating conditions. The lower the temperature, the longer the retention time. We operate at 55 ºC for 20 days. A part from methane and CO2, nitrogen, H2S, and NH3 are produced (Japaraju, P., Rintala, J. 2013). Thus, in order to compute the biogas composition a mass balance is performed considering the composition of the different manure sources:

 (1)

Where the typical composition, Yi,  of the biogas is given by the following bounds:

0.7YCH40.5

0.3YCO20.5

0.02YN20.06 (2)

0.005YO20.16

YH2S0.002

9·10-5 YNH31·10-4

The contact between biogas and the liquid residue results in biogas saturated with water. Gas moisture is computed using Antoine correlation as per Eq. (3). The flow of dry biogas is determined using Eq (4). To compute the power in the compressor, we need to determine the molar mass of the biogas as in Eq. (5). The mass flow rate of each component is computed from its molecular weight and the total mass flow rate, Eqs. (6)-(7).

 (3)

 (4)

 (5)

 (6)

 (7)

The lower and upper limits for the generation of biogas are given by Eq. (8) (Al Seadi et al., 2008)

0.20Vbiogas,waste 0.50;

0.10wMS,Waste 0.20; (8)

0.50wVSB,Waste 0.80;

The mass of waste that does not leave as biogas constitutes the digestate as follows. (Al Seadi et al 2008):

 (9)

Each manure type has its own composition Defra (2011).

620

0.005wN/Waste0.047;

0.005wNorg/ Waste 0.036;

0.008wP/ Waste 0.013; (10)

0.033wK/ Waste  0.1;

 (11)

Atom mass balances are performed to compute the products of the reactors. We consider balances for carbon, organic nitrogen (Norg), inorganic nitrogen (N), phosphate and potassium. The carbon either leaves in the form of CO2 or CH4 with the gas or as part of the waste in the digestate, Eq. (12). The organic nitrogen in the digestate is given by the fraction of organic nitrogen in the digestate minus the nitrogen released as gas, Eq (13). Similarly, the inorganic nitrogen that is not used to produce ammonia that accompanies the gas or is left as residue is computed using the values above, Eq. (14). P and K directly leave the reactor as part of the digestate, Eqs. (15)-(16). The rest that is not accounted for is assumed to be a residual part leaving the reactor with the digestate.

 (12)

 (13)

 (14)

 (15)

 (16)

 (17)

 (18)

The energy balance to the digester is as follows:

 (19)

The digestate is further conditioned.

**S.2.-H2S removal. ZnO**

Since biogas is burned for power production, any sulfur compound would potentially produce SO2. We can avoid it by removing theH2S. A reactive bed of Fe2O3 that operates at 25-50 ºC is used. The actual removal is carried out following the chemical reaction below (Ryckebosch et al., 2011).



Thus, the model of this unit is based on a mass balance based on the stoichiometry of the reaction assuming 100% conversion. The bed can be regenerated using oxygen (Ryckebosch et al., 2011).



**S.3.- CO2, NH3 and H2O removal (PSA)**

The flue gas from the gas turbine is to be used as heat source to produce steam for the steam turbine. Therefore, it is interesting that the stream has high temperature. CO2 is removed from biogas using a packed bed of zeolite 5A operating at 25ºC and 4.5 bar. To secure continuous operation, two adsorbent beds operate in parallel so that while one is in adsorbent mode, the second one is under regeneration. We assume a recovery of 100% for NH3 and H2O (because of their low total quantities in the biogas, in general), 95 % for CO2 and 0% for any other gas of the mixture [22, 23].

**S.4.- Brayton cycle**

The process consists of a three stage polytropic compressor with intercooling. Each compressor s modelled assuming polytropic behavior using Eqs. (20) - (21) to compute the exit temperature and the power required for each stage. After each compression stage, intercooling is used to reduce the power input. The polytropic coefficient, k, is taken to be 1.4 based on an offline simulation using CHEMCAD®. The efficiency of the compressor is assumed to be 85 % (Moran and Shapiro, 2003). A maximum compression ratio of 40 for air is used, based on typical achievements (Janet 1997). The intercooling stage is modeled as simple energy balance to compute the cooling required to cool down the gas to the initial temperature of the previous compressor.

 (20)

 (21)

The combustion of the biogas, see reactions below, heats up the mixture. We use an excess of 20 % of air with respect to the stoichiometry and assume 100 % conversion of the reaction.



The material balance is based on the stoichiometry of the chemical reaction stated above and an energy balance is used to compute temperature of the gases exiting the gas turbine as given by eq. (22):

 (22)

The hot flue gas is expanded in the gas turbine to generate power. Eqs. (39) and (49) are used to model the performance of the gas turbine. The polytropic coefficient is taken to be 1.3, also based on an offline simulation using CHEMCAD ®, with an efficiency of 85 % (Moran and Shapiro, 2003). Finally, the exhaust gas is cooled down and used to generate high pressure steam to be fed to the Rankine cycle.

**S.5.- Rankine cycle**

The steam is generated in a system of heat exchangers. Two alternatives are evaluated:

A) Only a fraction of the flue gas from the gas turbine is used to produce the high pressure steam fed to the steam turbine. The rest of the gas is used for the regeneration step.

B) The entire flue gas is used to heat up the saturated steam before feeding it to the high pressure turbine. Next, it is used to reheat the expanded steam before feeding it to the medium pressure turbine

In the second body of the turbine, part of the steam is extracted at a medium pressure and it is used to heat up the condensate. The rest of the steam is finally expanded to an exhaust pressure, condensed and recycled. The flue gas is used for heating up and evaporating this stream. Due to the size of the plants and their typical location, a farm, it is expected that a lagoon is used to condensate the working fluid. Each unit is modeled using mass and energy balances as well as thermodynamic properties (Martín and Martín, 2013; Vidal and Martín, 2015).

The enthalpy and entropy of steam as a function of the temperature and pressure are correlated as in previous work (Martín and Martín, 2013; Vidal and Martín, 2015). The equations can be found in the appendix below. Therefore, the stream exiting the first body can be calculated using Eqs. (23)-(28), assuming an isentropic efficiency, s, of 0.9.

 (23)

Where

 (24)

T\* represents the isentropic temperature after the expansion computed as follows::

 (25)

We make sure that the output of the turbine is superheated steam by maintaining its temperature above the one that corresponds to saturation for the pressure of the stream.

 (26)

 (27)

The energy that is obtained in the steam expansion in the first turbine is given by Eq. (28):

 (28)

The stream, as superheated vapor, is heated up again in HX5 using a fraction of the exhaust gas from the gas turbine, Eq. (29), or the entire flow depending on the flowsheet configuration, Eq. (30). Next, the superheated steam is fed to a second turbine. HX5 is modeled using Eq. (29)-(31)

 (29)

 (30)

 (31)

In the second turbine there is another expansion to a lower pressure. Part of the stream will be sent to HX7, while the rest is used in the third body of the turbine, where it is expanded to a pressure below atmosphere, see Eq. (32); this pressure ranges from 0.05 bar to 0.31 bar in the literature (Vidal and Martín, 2015). The second and third bodies of the turbine are calculated similarly to the first one, assuming 0.9 isentropic efficiency in all stages.

 (32)

The stream extracted from the medium pressure turbine is sent to HX7, where it will be used to reheat the liquid obtained after condensing the exhaust of the third body of the turbine. The exhaust of the low pressure turbine is assumed to be saturated vapor. This stream is condensed in HX6:

 (33)

This energy must be removed in the cooling system. We assume that a lagoon is used to cool down the water used to condense the saturated steam before reuse. This part is not included in the model. When mixing the exhaust of the second turbine with the compressed liquid from HX6, we must bear in mind that the outlet should be liquid since it is going to be compressed and heated up as a liquid in HX8. Eq. (34) ensures this fact:

 (34)

Where Tturb2min is the saturated temperature at the pressure of the exhaust of the second body of the turbine calculated using Antonine vapor pressure correlation.

**Nomenclature**

**Sets**















Unit:

**Parameters**

: specific clarifier area (m2 / (ton·day))

: work days per year

: particle diameter (m)

: Maximum diameter of *unit (m) /40m Clarfier,1.25 m Centrifuge /*

: equilibrium ion activity product

: work hours per day

: hydraulic retention time of *unit* (s)

: molecular weight of component (kg/kmol)

**: metal/phosphorus molar ratio in coagulation process

: price of the component (€/kg)

: gravity acceleration (m2/s)

= polytropic coefficient (1.4)

: kinetic constant /3.42·10-3 s-1 / (s-1)

: agitators specific power consumed ( HP / 1000 USgallon)

: precipitation agent *j* per total solids mass ratio

: Compressor’s efficiency (0.85)

: Isentropic efficiency (0.9)

: *i* component separation yield using in the process the element *j*

: atmospheric pressure (1 bar)

: atmospheric temperature (25 ºC)

: ideal gas constant (8.314 J/mol·K)

: specific heat capacity of water (4.18 kJ/kg·ºC)

: parameter dependent of the phases number in the FBR

: *component* density (kg/m3)

: viscosity of component (kg/(m·s))

**Variables**

: parameter which takes the value 0 when is 0 and 1 if is not equal to 0

: Arquimedes number for liquid

: area of *unit* (m2)

: benefits or losses obtained with *technology*

: carbon to nitrogen molar ratio

: equilibrium concentration (kmol/m3)

: initial concentration (kmol/m3)

: cost of *unit*

: concentration of *component* in the *unit* inlet stream (kgcomponent/ kgtotal)

**: cost of chemicals for *technology*

: diameter of *unit*

: thickness of *unit*

: equilibrium constant of component *j* at temperature T.

:mass flow of *component* in the *unit* inlet stream (kg/s)

: maximum mass inlet flow admitted by a single *unit* (kg/s)

: mass inlet flow used in the design of *unit* (kg/s)

: fixed cost of *technology*

: recovered matter total mass flow (kg/s)

: mass flow from stream from unit to unit1 (kg/s)

: mass flow of component J from unit to unit1 (kg/s)

: enthalpy of the stream at the state b from the stream from unit to unit1 (kJ/kg).

: enthalpy of the stream at the if the expansion is isentropic (kJ/kg).

: molar fraction of component *j* in the liquid phase of equilibrium system *i*.

: Potassium index of fertilizer.

: length of *unit*

: nitrogen contained in ammonia.

: nitrogen contained in organic matter.

: number of *units* used in the process

: total mol flow from stream from unit to unit1 (kmol/s).

: nitrogen index of fertilizer.

: inlet pressure to compressor (bar).

: outlet pressure of compressor (bar).

: saturation pressure of pure component *j* at temperature T (bar).

: vapor pressure (bar)

: phosphorous index of fertilizer.

: inlet pressure to body *i* in the turbine (bar)

**: power of *unit*

: heat exchanged in unit (kW).

: carbon to nitrogen ratio in *k*.

: carbon to nitrogen ratio in fertilizer.

: rate of evaporation in equilibrium system *i*.

: rest of the elements contained in the biomass.

: Reynolds number for liquid in minimum fluidization conditions

: entropy the stream at the state b for the stream from unit to uni1 kJ/kg.K

: saturating temperature at exit of body *i* (ºC)

: temperature of the stream from unit to unit 1 (ºC)

: bubble point temperature of equilibrium system *i* (ºC).

: average temperature in equilibrium system *i* (ºC).

: inlet temperature to compressor (ºC).

: outlet temperature of compressor (ºC).

: time (s)

: terminal velocity (m/s)

: fluid velocity (m/s)

: minimum fluidization velocity (m/s)

: molar fraction of component *j* in the vapor phase of equilibrium system *i*.

: biogas volume produced per unit of volatile solids (VS) (m3biogás/kgVS/k) associated to *k*.

: volume of *unit*

: weight of *unit*

: dry mass fraction of *k* (kgDM/k/kg).

: dry mass fraction of volatile solids out of the dry mass of *k* (kgVS/k/kgDM/k).

: dry mass fraction of C in k (kgC/k/kgDM/k).

: dry mass fraction of Nam in k (kgNam/k/kgDM/k).

: dry mass fraction of Norg in k (kgNorg/k/kgDM/k).

: dry mass fraction of P in k (kgP/k/kgDM/k).

: dry mass fraction of K in k (kgK/k/kgDM/k).

: dry mass fraction of the rest of the elements contained in k (kgK/k/kgMS/k).

: power produced or consumed in unit (kW).

: mass fraction of component *a* in the biogas

: binary variable to evaluate the element *j*

: specific saturated moisture of biogas

: molar fraction of component a in the dry biogas.

: Heat of the anaerobic digestion’s reaction (kW).

: heat of combustion of component *k* (kW).

: heat of combustion of component *e* (kW).

: heat of combustion of dry digestate (kW)

: heat of formation of component *h* at temperature T(unit,unit1) (kW)

: objective function

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**Appendix**

Temperature in ºC

***Compressed liquid***

H(kJ/kg)=4.2921\*(TEMPERATURE) + 4.1269

S (kJ/(kg K))=1.1902\*10 -5\*(TEMPERATURE)3 - 3.7465\*10-3\*(TEMPERATURE)2 + 4.5352\*(TEMPERATURE) + 0.64547

***Saturated liquid***

H(kJ/kg)=3.6082\*10-12\*(TEMPERATURE) 6 - 3.4120\*10-9\*(TEMPERATURE)5 +

1.2303\*10-6\*(TEMPERATURE)4 - 2.0306\*10-4\*(TEMPERATURE)3 +

1.5552\*10-2\*(TEMPERATURE)2 + 3.7216\*(TEMPERATURE) + 3.0035

S (kJ/(kg K))= 1.0372\*10-12\*(TEMPERATURE)5 - 8.6494\*10-10\*(TEMPERATURE)4 +

2.8965\*10-7\*(TEMPERATURE)3 - 5.6730\*10-5\*(TEMPERATURE)2 +

1.6802\*10-2\*(TEMPERATURE) - 2.1997\*10-2

***Saturated Vapor***

H (kJ/kg)=-6.5690\*10-12\*(TEMPERATURE)6 +

6.3049\*10\*\*(-9)\*(TEMPERATURE )5 - 2.3080\*10-6\*(TEMPERATURE)4 +

3.8339\*10\*\*(-4)\*(TEMPERATURE)3 - 3.0632\*10-2\*(TEMPERATURE)2 +

2.7553\*(TEMPERATURE) + 2.4957\*103

S (kJ/(kg K))=

-2.0373\*10-12\*(TEMPERATURE)5 + 1.8589\*10-9\*(TEMPERATURE)4 -

7.1901\*10-7\*(TEMPERATURE)3 + 1.6112\*10-4\*(TEMPERATURE)2 -

2.8904\*10-2\*(TEMPERATURE) + 9.1915

***Superheated steam (Up to 10 bar)***

H (kJ/kg)= ( -0.0000063293\*(Pressure(bar)) + 0.00033179)\*(TEMPERATURE)2+(0.0124\*(Pressure(bar)) + 1.8039)\*(TEMPERATURE)+(-6.0707\*(Pressure(bar))+2504.6)

S (kJ/(kg K))=

0.000000000942\*(TEMPERATURE)3-0.00000309\*(TEMPERATURE)2+0.00524\*(TEMPERATURE)+(6.8171\*((Pressure(bar))) (-0.069455))

***Superheated steam (10 bar -150bar)***

H (kJ/kg)= (-0.00000000000011619\*(Pressure(bar))2 - 0.0000000000087596\*(Pressure(bar)) - 0.00000000022611)\*(TEMPERATURE) 4+

(0.0000000004298\*(Pressure(bar))2 + 0.00000003276\*(Pressure(bar)) + 0.0000007313)\*(TEMPERATURE)3+

(-0.0000005801\*(Pressure(bar))2 - 0.000046\*(Pressure(bar)) - 0.0005009)\*(TEMPERATURE)2+

(0.0003383\*(Pressure(bar))2 + 0.02947\*(Pressure(bar)) + 2.195)\*(TEMPERATURE)+

(-0.072042\*(Pressure(bar))2 - 7.7877\*(Pressure(bar)) + 2440.8)

S (kJ/(kg K))= (0.000000000015719\*(Pressure(bar)) + 0.00000000074013)\*(TEMPERATURE)3+

(-0.00000000010074\*(Pressure(bar))2 - 0.000000030171\*(Pressure(bar)) - 0.0000028872)\*(TEMPERATURE)2+

(0.000000094914\*(Pressure(bar))2 + 0.000029097\*(Pressure(bar)) + 0.0050938)\*(TEMPERATURE)+

(0.000041223\*(Pressure(bar))2 - 0.028841\*(Pressure(bar)) + 5.9537)

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