Data in brief 29 (2020) 105212

Contents lists available at ScienceDirect

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Data Article

Comprehensive determination of input state variables dataset required for anaerobic digestion modelling (ADM1) based on characterisation of organic substrates

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ARTICLE INFO

Article history:
Received 28 October 2019
Received in revised form 8 January 2020
Accepted 23 January 2020
Available online 31 January 2020

Keywords:
ADM1 model
Fractionation
Organic substrates
Nitrogen content

ABSTRACT

This article contains the data of 11 organic substrates including physicochemical, biochemical and nutritional characterisations. Additionally, it includes for all substrates the data of organic matter fractionation into easily biodegradable, slowly biodegradable and inert fractions performed with anaerobic respirometry method. Finally, based on physicochemical characterisations and organic matter fractionation, a detailed methodology for the determination of input state variables required for the anaerobic digestion model N°1 (ADM1) was presented and the dataset for all substrates is provided. An example of calculation for one substrate illustrates the methodology for the determination of these variables. Data provided in this article could be useful to any person interested in modelling anaerobic digestion and particularly co-digestion. Data could be also used for implementation of a database for anaerobic digestion modelling.

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https://doi.org/10.1016/j.dib.2020.105212

Specifications Table

Subject	Renewable Energy, Sustainability and the Environment Ecological Modelling Environmental Engineering
Specific subject area	Detailed characterisation and fractionation of organic wastes required as input state variable for anaerobic digestion model N°1 (ADM1)
Type of data	Tables
How data were acquired	Data was acquired using classical physico-chemical analyses and instruments including: pH probe, oven drying, furnace calcination, mineralisation, titration, ionic and gas chromatography, NMR. In addition, characterisation data were used to calculate the fractionation needed as input state variable of ADM1.
Data format	Raw Analysed
Parameters for data collection	Characterisation data were collected from substrates from the agro-industrial, agricultural and urban sectors typically used on the anaerobic digestion process. Eleven substrates were characterised including *slurry, greases, primary sludge, secondary sludge, vinasses, biowaste, feed residues, silage, horse feed, manure* and *grape marc*. A large physicochemical, biochemical and nutritional characterisation was performed on these substrates. The input state variables for ADM1 were determinate using characterisation data.
Description of data collection	After collection, each sample was stored at −20 °C until analyses. Frozen solid wastes were ground to obtain a homogenous sample. Extractions and centrifugation were performed in order to determine soluble characteristics. Input state variables were then calculated.
Data source location	Institution: All substrates were collected by Irstea-OPAALE and INRA-LBE Region: Mainly nearby to Rennes and Narbonne cities Country: France Latitude and longitude for collected samples: Rennes: 48°06′53'' N 1°40′46″ W Narbonne: 43°11′02″N 3°00′05″ E
Data accessibility	With the article

Value of the Data

- Data in this paper provides a robust characterisation of various organic wastes and a comprehensive determination of input state variables required for anaerobic digestion model N°1 (ADM1)
- Data in this paper can be used by researchers, students, private organisations, any person using ADM1
- Data in this paper can be used to compare and check characterisation of substrates and fractionation used for ADM1

1. Data

The dataset contains the characterisation and fractionation of organic substrates required as input state variable for anaerobic digestion model N°1 (ADM1). The list and the description of substrates studied in this article are presented in Table 1. Table 2 shows the main physicochemical, biochemical and nutritional characteristics of the organic substrates. These characteristics are used to determine input state variables for ADM1. Table 3 shows the fractionation of the organic matter determined using a simplified anaerobic digestion model combined with the methane production rate curves obtained from the anaerobic respirometry test. The simplified model used to generate data provided in Table 3 is described in the subsection "Organic matter fractionation" of the "Experimental Design, Materials, and Methods" section. Table 4 shows the results of the calculation of nitrogen content of inert fractions (N_i) to obtain an accurate value of input organic nitrogen (N_{org}). Table 5 and Table 6 provide the dataset of input state variables required for the ADM1. Table 5 provides the soluble fractions while Table 6 provides the particulates fractions. These variables were determined using the detailed methodology described in the Experimental Design, Materials, and Methods section.

Table 1
Substrates description.

Substrate	Description
Slurry	Centrifuged pig slurry
Greases	Slaughterhouse flotation greases
Sludge I	Primary sewage sludge from municipal wastewater treatment plant
Sludge II	Secondary sewage sludge from municipal wastewater treatment plant
Vinasses	Liquid vinasses from wine distilleries
Biowaste	Kitchen waste and leftovers of the dishes served from a collective catering establishment
Feed residues	Livestock feed residues
Silage	Corn silage
Horse feed	Commercial horse feed
Manure	Cattle manure with low straw content
Grape marc	Solid remains of grapes pressing from wine distilleries

2. Experimental design, materials, and methods

2.1. Physicochemical and biochemical characterisation of organic substrates

Preparation of substrates and main physicochemical and biochemical characterisation methods used in this article were described by Fisgativa et al. [1]. Briefly, pH was measured on liquid phases or extractions of substrates using a pH probe. TS, VS and COD were determined following standard methods (EN12880-12879, NF T90-101). Total TKN, total NH_4^+, total phosphorus and total potassium were determined with the standard methods (NF EN 13342, NF EN ISO 11885). VFA were determined by high pressure liquid chromatography (HPLC) on liquid phases or liquid extractions of substrates as explained by Girault et al. [2].

Biochemical methane potential (BMP) was performed using raw substrates. Inoculum was collected from a well-established CSTR running with a hydraulic retention time of 24 days and fed with horse feed and centrifuged slurry. BMP bottles were filled using a ratio of $1gVS_{inoculum}$:$1gVS_{substrate}$. Before incubation, the head space of the BMP bottles was renewed with N_2. The bottles were incubated at 38 °C for about 40 days. Gas production was recorded and gas samples were taken daily the first week and afterwards two to three times per week until the end of the experiment. Gas samples were analysed to determine CH_4 and CO_2 concentrations by gas chromatography using the method described by Lucas et al. [3].

Lipids content was determined on dry substrates using nuclear magnetic resonance (NMR) as described by Picard et al. [4]. Protein was determined considering the organic nitrogen content (N_{org}) (N_{org} content = TKN content − NH_4^+ content) and a ratio protein to N_{org} of 6.25. The calculation of COD proportion of proteins and lipids was based on methodology described by Girault et al. [2], using the following equations:

$$proteins\ (\%COD) = 100 * \frac{proteins\left(\frac{g_{proteins}}{kgVS}\right) * 1.42\left(\frac{gO_2}{g_{proteins}}\right)}{COD\left(\frac{gO_2}{kgVS}\right)}$$

$$lipids\ (\%COD) = 100 * \frac{lipids\left(\frac{g_{lipids}}{kgVS}\right) * 2.86\left(\frac{gO_2}{g_{lipids}}\right)}{COD\left(\frac{gO_2}{kgVS}\right)}$$

Table 2
Physicochemical, biochemical and nutritional characterisation mainly used to determine input state variables for ADM1.

Substrates	pH	TSa	VS	CODtot	TC	TIC	TKN	NH4+	Ptot	Ktot	Lipids	Proteins	Carbohydrates	BMP	BNP	VFA
		gTS· kgWW-1	gVS· kgWW-1	gO2· kgWW-1	gC· kgWW-1	gC· kgWW-1	gN· kgWW-1	gN· kgWW-1	gP· kgWW-1	gK· kgWW-1	%COD	%COD	%COD	NLCH4· kgWW-1	gN· kgWW-1	gVFA· kgWW-1
Slurry	8.60	10.0	4.4	5.0	4.1	1.1	1.9	1.5	0.10	1.74	10.7%	68.4%	21.0%	0.4	0.28	0.01
Greases	5.50	146.3	128.2	342.9	84.0	0.4	2.8	0.3	0.54	0.25	64.0%	6.4%	29.5%	107.3	1.02	1.76
I Sludge	5.44	57.3	46.0	79.1	25.7	0.7	1.8	0.1	0.40	0.20	26.0%	19.1%	54.9%	15.9	1.30	0.99
II Sludge	5.94	53.7	42.2	70.4	21.1	0.3	3.9	0.2	1.39	0.58	13.7%	46.1%	40.2%	7.8	2.61	0.09
Vinasses	4.63	171.3	126.6	221.0	73.8	3.6	5.9	0.1	0.75	5.97	15.2%	23.4%	61.4%	24.9	0.57	2.17
Biowaste	5.28	190.2	172.8	287.7	93.9	1.1	6.4	0.1	1.43	2.74	40.2%	19.4%	40.5%	81.6	5.86	0.25
Feed residues	6.19	802.0	761.1	993.8	353.2	1.0	21.2	0.8	3.65	5.16	9.6%	18.3%	72.1%	283.3	16.65	0.53
Silage	4.09	303.0	293.3	428.9	138.9	0.2	4.0	0.3	0.49	2.53	7.1%	7.8%	85.2%	118.6	1.44	6.98
Horse feed	5.78	891.1	801.1	1034	381.0	4.5	20.2	0.1	5.20	11.1	10.7%	17.3%	72.0%	288.4	16.14	0.40
Manure	8.54	191.3	155.7	243.1	79.6	1.2	5.2	0.8	1.22	9.02	4.7%	16.2%	79.1%	39.6	0.43	0.00
Grape marc	4.35	419.2	395.5	549.4	211.0	11.1	8.9	0.0	4.32	25.0	22.5%	14.2%	63.2%	44.0	0.43	0.42

[a] Acronyms used on this table are: TS - Total solids, VS- Volatile solids, COD_{tot} - Total chemical oxygen demand, TC - Total carbon content, TIC - Total inorganic carbon content, TKN - Total Kjeldahl nitrogen, BMP - Biochemical methane potential, BNP - Biological nitrogen potential, VFA- Volatile fatty acids, WW - Wet weight.

Table 3
Organic matter fractionation determined by anaerobic respirometry test.

Substrates	X_i	S_s	X_s	k_h	$\mu \cdot XB$
	$gO_2 \cdot kgWW^{-1}$	$gO_2 \cdot kgWW^{-1}$	$gO_2 \cdot kgWW^{-1}$	j^{-1}	j^{-1}
Slurry	3.82	0.40	0.81	0.25	0.08
Greases	0.00	92.7	250	0.45	0.15
I Sludge	0.33	2.49	76.3	0.44	0.17
II Sludge	29.8	16.2	24.5	0.27	0.13
Vinasses	115	28.5	77.0	0.54	0.27
Biowaste	41.0	108	139	0.18	0.13
Feed residues	157	184	653	0.21	0.11
Silage	75.0	19.7	334	0.37	0.16
Horse feed	247	476	311	0.19	0.17
Manure	146	3.27	93.4	0.08	0.10
Grape marc	366	181	2.08	0.003	0.24

Table 4
Calculated values of nitrogen content of inert fractions.

Substrates	N_i
	$kmoleN \cdot kgO_2^{-1}$
Slurry	0,007
Greases	0,004[a]
I Sludge	0,090
II Sludge	0,003
Vinasses	0,003
Biowaste	0,001
Feed residues	0,002
Silage	0,002
Horse feed	0,001
Manure	0,002
Grape marc	0,002

[a] Default value.

Finally, the COD proportion of carbohydrates was determined as the remaining COD fraction after removal of the lipids and proteins from total COD.

$$carbohydrates\ (\%COD) = 100 - proteins\ (\%COD) - lipids\ (\%COD)$$

Biological nitrogen potential (BNP) was performed as described by Bareha et al. [5]. In brief, the BNP experimental conditions were similar to the BMP experiments with an additional ammonium concentration monitoring. The main difference is that in the BNP tests the inoculum was previously centrifuged at 12,100g for 20 min and the supernatant was removed in order to reduce the initial ammonium concentration and, then, to be able to monitor ammonium variations during digestion. The lost buffering capacity of centrifuged inoculum was restored suspending the remained pellet in a $KHCO_3$ 10 g L^{-1} + $NaHCO_3$ 10 g L^{-1} solution. The addition ratio of inoculum and substrate to the bottles was similar than for BMP ($1gVS_{inoculum}$:$1gVS_{substrate}$). The bottles were also incubated at 38 °C for about 40 days. Gas samples were taken and analysed similarly than for BMP test. TKN and NH_4^+ analyses were performed at the beginning and at the end of the experiment. BNP value was then calculated as the difference between the initial and the final ammonium content, subtracting the ammonium content of blank corresponding to a digestion of the inoculum alone.

2.2. Anaerobic respirometry test

Anaerobic respirometry test was performed as descripted by Girault et al. [2]. Briefly, the same inoculum than for BMP was used. Cells of 1.2 L were filled with 1 L of inoculum and 5 gCOD of

Table 5
Set of ADM1 model soluble input state variables for all substrates.

Substrates	S_{su}	S_{aa}	S_{aglc}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	S_{ic}	S_{in}	S_i	S_{cat}	S_{an}
	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kM\ C \cdot m^{-3}$	$kM\ N \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$KM \cdot m^{-3}$	$KM \cdot m^{-3}$
Slurry	0.26	0.00	0.13	0.00	0.00	0.00	0.01	0.00	0.00	0.09	0.11	0.00	0.04	0.02
Greases	27.6	2.80	59.8	0.00	0.00	2.07	0.42	0.00	0.00	0.04	0.02	0.00	0.04	0.02
I Sludge	0.55	0.42	0.26	0.00	0.00	0.70	0.57	0.00	0.00	0.05	0.01	0.00	0.04	0.02
II Sludge	4.08	10.6	1.39	0.00	0.00	0.06	0.05	0.00	0.00	0.03	0.02	0.00	0.02	0.02
Vinasses	19.7	1.57	4.89	0.00	0.00	0.00	2.31	0.00	0.00	0.30	0.01	0.00	0.03	0.02
Biowaste	40.9	26.2	40.6	0.00	0.00	0.00	0.27	0.00	0.00	0.09	0.01	0.00	0.04	0.02
Feed residues	129	37.3	17.2	0.00	0.00	0.00	0.57	0.00	0.00	0.09	0.06	0.00	0.05	0.02
Silage	9.84	0.82	0.82	0.00	0.00	2.51	5.67	0.00	0.00	0.02	0.02	0.00	0.03	0.02
Horse feed	327	99.7	48.8	0.00	0.00	0.00	0.43	0.00	0.00	0.38	0.01	0.00	0.23	0.02
Manure	2.95	0.15	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.10	0.05	0.00	0.10	0.02
Grape marc	130	4.38	46.3	0.00	0.00	0.00	0.45	0.00	0.00	0.92	0.00	0.00	0.03	0.02

Table 6
Set of ADM1 model particulate input state variables for all substrates.

Substrates	X_c	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{aglc}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	X_i[a]
	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$	$kgO_2 \cdot m^{-3}$
Slurry	0.00	0.50	0.00	0.30	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
Greases	0.00	76.6	7.60	166	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.11
I Sludge	0.00	43.1	12.8	20.4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
II Sludge	0.00	6.3	16.0	2.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08
Vinasses	0.00	58.3	4.20	14.5	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.37
Biowaste	0.00	52.7	33.6	52.3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03
Feed residues	0.00	459	132	61.2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.27
Silage	0.00	296	13.9	24.6	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.17
Horse feed	0.00	214	65.0	31.9	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.28
Manure	0.00	84.2	4.30	4.90	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.29
Grape marc	0.00	1.5	0.10	0.50	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60

[a] X_i in this table correspond to the calculate particulate inert content using Ni value from Table 4.

substrate. The renewal of the atmosphere of the cells head space was carried out with a mixture of N_2 and CO_2 (70/30) to avoid decarbonation of the inoculum. The cells were continuously mixed at 1200 rpm and kept at 38 °C for 17 days. Gas production rate was continuously monitored and recorded by means of pressure sensors. Gas samples were taken twice a day during the first week and once a day during the second week of the experiment. Gas samples were analyses with the same methodology than for BMP.

2.3. Organic matter fractionation

To determine the fractionation of organic matter from substrates, a simplified anaerobic digestion model was used. For this purpose, three compartments were considered:

- An easily biodegradable and directly assimilable fraction (S_s)
- A slowly biodegradable fraction requiring previous hydrolysis before assimilation (X_s)
- An inert fraction (Xi)

According to the simplified anaerobic digestion model (Fig. 1), the inert fraction is not transformed while the X_s fraction is hydrolysed to S_s and the S_s fraction is consumed by anaerobic bacteria (X_B) producing CH_4. As the inoculum to substrate ratio is high, the growth and the decay of bacteria during the trial could be neglected leading to X_B constant during the experiment.

Then the processes can be simulated using the following equations:

$$\frac{dCH_4}{dt} = -(1-Y).\frac{dS_s}{dt}$$

$$\frac{dX_s}{dt} = -k_h.X_s$$

$$\frac{dS_s}{dt} = -\frac{1}{Y}.\frac{S_s}{(S_s+K_s)}.\mu X_{B\ initial} + \frac{dX_s}{dt}$$

With K_s: half-saturation constant of S_s.
μ: bacterial growth rate.
k_h: hydrolysis rate coefficient.
Y: yield of biomass.

Using these equations and the methane production rates (MPR), corresponding to $\frac{dCH_4}{dt}$, obtained from the anaerobic respirometry tests, the fractions X_s and S_s as well as k_h were determined for each substrate by mathematical optimization (Minimizing last-squares between experimental MPR and $\frac{dCH_4}{dt}$ from the model combined with Monte Carlo method for parameters and fractions). For this optimization, we considered that:

- The sum of the biodegradable fractions, *i.e.* $S_s + X_s$, is equal to the BMP calculated on COD basis. Consequently, the inert fraction X_i is equal to the total COD minus the BMP.
- The fraction S_s must be equal to or greater than the VFAs.

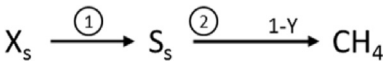

Fig. 1. Description of the anaerobic digestion processes of the model used to fractionate organic matter: 1) Hydrolysis of X_s to S_s, 2) Consumption of S_s by bacteria (X_B) and production of CH_4.

- There is still recalcitrant organic matter left in the inoculum. As a result, an additional hydrolysis process was added to the inoculum alone. This hydrolysis process is calculated from similar experiment without substrate addition.
- As X_B is considered constant during the experiment and equal to $X_{B.initial}$, a new parameter called μX_B corresponding to $\mu.X_{B.initial}$ was considered as each parameter was not identifiable alone.
- The initial K_s and μX_B parameters used for optimization were the result of a previous optimization using kinetic MPR from similar experiments with acetate addition. The variation ranges used for optimization for these parameters were 1–10 and 1 to 3, respectively.

2.4. Determination of input variables required for ADM1 modelling

Biodegradable fractionation of organic matter obtained from anaerobic respirometry experiments Table 3 and lipid/carbohydrate/protein fractionation (Table 2) are the basis for the determination of input variables. Indeed, the fractions S_s and X_s must be split to serve as an input to the ADM1 model. In addition, other physicochemical parameters must be adapted for use in the model. The input variables of the model are as follows:

- The S_s fraction was decomposed into the soluble materials considered by the model, namely: sugars (S_{su}), amino acids (S_{aa}), long chain fatty acids (S_{lcfa}), acetic acid (S_{ac}), propionic acid (S_{pr}), butyric acid (S_{bu}) and valeric acid (S_{va}).
- The X_s fraction was also decomposed into the slowly degradable fractions considered by the model, namely: carbohydrates (X_{ch}), proteins (X_{pr}) and lipids (X_{li}) slowly biodegradable.
- The remaining soluble variables were determined by characterization or by following recommended values, namely: soluble hydrogen (S_{h2}), soluble methane (S_{ch4}), inorganic carbon (S_{ic}), inorganic nitrogen (S_{in}), soluble inert particles (S_I), cations (S_{cat}) and anions (S_{an}).
- Also, the remaining particulate variables were determined by characterization or by following recommended values, namely: composites (X_c), particulate inerts (X_I) and biomass responsible for the degradation of: sugars (X_{su}), amino acids (X_{aa}), acetic acid (X_{ac}), propionic acid (X_{pro}), acids of 4 or more carbons (X_{c4}), LCFA (X_{lcfa}) and hydrogen (X_{h2}).

The decomposition of the S_s and X_s fractions was carried out taking into account the characterisation of the substrates (Table 2). In addition, the BNP value was used in the determination of the input variables to include the notion of nitrogen biodegradability. With these elements in hand, the progressive determination of the input variables was carried according to the following steps. The example of the calculation of the input variables for the “Horse Feed” substrate is given for greater clarity:

1. Biodegradable nitrogen was calculated as follows:

$$(X_{pr} + S_{aa}) = \frac{BNP}{N_{aa} * M_N}$$

Where, X_{pr} and S_{aa} were expressed in $kgO_2.m^{-3}$, BNP in $kgN.m^{-3}$, N_{aa} is the nitrogen content of amino acids and proteins expressed in $kmoleN.kgO_2^{-1}$ (0.007 according to Batstone et al. [6]) and M_N is the molecular weight of nitrogen (14 $kgN.kmole^{-1}$). For the Horse Feed:

$$(X_{pr} + S_{aa}) = \frac{16.1}{0.007 * 14} = 164.7\ kgO_2.m^{-3}$$

2. This sum $(X_{pr} + S_{aa})$ was split into X_{pr} and S_{aa} proportionally to quantity of X_s and S_s in the biodegradable fraction as follow:

$$(X_{pr} + S_{aa}) * \frac{X_s}{(X_s + S_s)} = X_{pr}$$

$$(X_{pr} + S_{aa}) * \frac{S_s}{(X_s + S_s)} = S_{aa}$$

In the case of Horse Feed, X_s represents 39.5% of the organic biodegradable fraction and S_s represents 60.5%, obtaining:

$$X_{pr} = 164.7 * 39.5\% = 65.0\ kgO_2.m^{-3}$$

$$S_{aa} = 164.7 * 60.5\% = \ 99.7\ kgO_2.m^{-3}$$

3. Then, by subtracting the value of the X_{pr} from X_s, the fraction of $X_{s\text{-}pr}$ is obtained, corresponding only to carbohydrates and fats. To obtain the fractions X_{ch} and X_{li}, the distribution of fats and carbohydrates in relation to the COD without taking into account proteins, as follow:

$$\%Carbohydrates\ (\%\ COD_{-proteins}) = \frac{Carbohydrates\ (\%COD)}{Carbohydrates\ (\%COD) + Lipids\ (\%COD)}$$

$$\%Lipids\ (\%\ COD_{-proteins}) = \frac{Lipids\ (\%COD)}{Carbohydrates\ (\%COD) + Lipids\ (\%COD)}$$

Then:

$$X_s - X_{pr} = (X_{ch} + X_{li})$$

$$(X_{ch} + X_{li}) * \%Carbohydrates\ (\%\ COD_{-proteins}) = X_{ch}$$

$$(X_{ch} + X_{li}) * \%Lipids\ (\%\ COD_{-proteins}) = X_{li}$$

In the case of the Horse Feed, the percentage of carbohydrate COD (excluding protein) is 87.0% and the percentage for fat is 13.0%, therefore:

$$X_s - X_{pr} = 310.7 - 65.0 = 245.7\ \ kgO_2.m^{-3} = (X_{ch} + X_{li})$$

$$X_{ch} = 245.7 * 87.0\% = 213.8\ kgO_2.m^{-3}$$

$$X_{li} = 245.7 * 13.0\% = 31.9\ gkO_2.m^{-3}$$

At this stage, the repartition of X_s was completed.

4. The remaining fractioning of the S_s follows a similar logic. Hence, subtracting the value of S_{aa} from the S_s gives the fraction $S_{s\text{-}aa}$ corresponding only to VFA, LCFA and sugars. The VFA content was based on the chemical characterisation. The remaining $S_{s\text{-}aa\text{-}VFA}$ (after subtraction of VFAs) was fractionated with the same percentages of carbohydrates and lipids (% always in COD and without taking into account proteins) to obtain the S_{su} and S_{fa} fractions:

$$S_s - S_{aa} - S_{ac} - S_{pr} - S_{bu} - S_{va} = \left(S_{su} + S_{fa}\right)$$

$$\left(S_{su} + S_{fa}\right) * \%Carbohydrates\ (\%COD) = S_{su}$$

$$\left(S_{su} + S_{fa}\right) * \%Lipids\ (\%\ COD) = S_{fa}$$

For Horse Feed, the acetic acid content is 0.4 $kgO_2.m^{-3}$. Propionic, butyric and valeric acids were not detected. The calculation would therefore be:

$$476.4 - 99.7 - 0.4 - 0.0 - 0.0 - 0.0 = 376.3\ kgO_2.m^{-3} = \left(S_{su} + S_{fa}\right)$$

$$S_{su} = 376.3 * 87.0\% = 327.4\ kgO_2.m^{-3}$$

$$S_{fa} = 376.3 * 13.0\% = 48.8\ kgO_2.m^{-3}$$

The repartition of S_s was completed.

5. The remaining soluble variables were determined as follows:
   - The variables S_{h2}, S_{ch4} and S_I were considered nil.
   - The variable S_{ic} corresponds to the inorganic carbon content (0.38 $kmoleC.m^{-3}$ for horse feed).
   - The variable S_{in} corresponds to the NH_4^+ content (0.01 $kmoleN.m^{-3}$ for horse feed).
   - The variable S_{an} was set at 0.02 $kmole.m^{-3}$
   - The variable S_{cat} was calculated according to S_{an}, pH and ions of VFA, carbonates and inorganic nitrogen as follows:

$$S_{cat} = S_{hco3} + \frac{S_{ac\_ion}}{64} + \frac{S_{pro\_ion}}{112} + \frac{S_{bu\_ion}}{160} + \frac{S_{va\_ion}}{208} + \frac{K_w}{S_{h+}} + S_{an} - S_{in} + S_{nh3} - S_{h+}$$

Where 64, 112, 160 and 208 are the grams of oxygen needed to degrade acetic, propionic, butyric and valeric acid respectively.

The different components of the equation have been calculated as follows:

$$S_{h+} = 10^{-pH}$$

$$S_{hco3} = \frac{K_{a\_co2} * S_{ic}}{(K_{a\_co2} + S_{h+})}$$

$$S_{ac\_ion} = \frac{10^{-pKa\_ac} * S_{ac}}{\left(10^{-pKa\_ac} + S_{h+}\right)}$$

$$S_{pro\_ion} = \frac{10^{-pKa\_pro} * S_{pro}}{\left(10^{-pKa\_pro} + S_{h+}\right)}$$

$$S_{bu\_ion} = \frac{10^{-pKa\_bu} * S_{bu}}{\left(10^{-pKa\_bu} + S_{h+}\right)}$$

$$S_{va\_ion} = \frac{10^{-pKa\_va} * S_{va}}{\left(10^{-pKa\_va} + S_{h+}\right)}$$

$$S_{nh3} = S_{in} - \frac{S_{h+} * S_{in}}{(K_{a\_in} + S_{h+})}$$

Where, the pK_a values used were: acetic = 4.76 M, propionic = 4.88 M, butyric = 4.82 and valeric = 4.86 M. The value of K_{a_co2} was 4.94E-07 and the value of K_{a_in} was 1.11E-09.

Making these calculations, the S_{cat} for Horse Feed corresponds to 0.23 kmole.m^{-3}.

6. The remaining particulate variables were determined as follows: composites (X_c) and all biomasses (X_{su}, X_{aa}, X_{ac}, X_{pro}, X_{c4}, X_{lcfa} and X_{h2}) were considered nil.
7. As previously mentioned for the simplified model, the inert fraction X_i is equal to the total COD minus the BMP, i.e. Ss + Xs.
8. A nitrogen content of inert (N_i) was calculated from X_i. This value of the stoichiometry parameter of the N_i was calculated for each substrate to be consistent with the measured N_{org} content. Indeed, the measured N_{org} content includes inert nitrogen in different proportions depending on the substrate, which is not taken into account by the default N_i parameter (0.004). The process of calculating N_i for each substrate and the variations it produces are therefore as follows:
   - The biodegradable nitrogen ($N_{org,bio}$) of the model was calculated without taking into account X_i and S_i.
   - The $N_{org,bio}$ would therefore be calculated as the sum of the nitrogen content of the variables: S_{aa}, X_c, X_{pr}, X_{su}, X_{aa}, X_{lcfa}, X_{c4}, X_{pro}, X_{ac}, X_{h2}.

- The nitrogen content for composites fraction (X_c) was 0.003 kmoleN.kgO_2^{-1}, for amino acids and proteins fractions (S_{aa}, X_{pr}) was 0.007 kmoleN.kgO_2^{-1} and for bacteria (X_{su}, X_{aa}, X_{lcfa}, X_{c4}, X_{pro}, X_{ac}, X_{h2}) was 0.006 kmoleN.kgO_2^{-1}.
- This $N_{org,bio}$, without X_i or S_i, was subtracted from the N_{org} measured at substrates and divided by the sum of the value of X_i of the substrates calculates by anaerobic respirometry. This relationship allows us to obtain N_i from each substrate:

$$N_{org,\ mesured} - N_{org,bio} = N_{org,inert}$$

$$\frac{N_{org,\ inert}}{X_i} = N_{i\ modified}$$

By performing these processes, the determination of the input variables of the ADM1 model was complete and could be used for modelling.

Acknowledgments

This study is part of the MAPPED project (2017–2019) N°1782C0076, which is supported by the French Environment & Energy Management Agency (ADEME).

Conflicts of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.dib.2020.105212.

References

[1] H. Fisgativa, C. Marcilhac, R. Girault, M.-L. Daumer, A. Trémier, P. Dabert, F. Béline, Physico-chemical, biochemical and nutritional characterisation of 42 organic wastes and residues from France, Data Brief 19 (2018) 1953–1962.
[2] R. Girault, G. Bridoux, F. Nauleau, C. Poullain, J. Buffet, J.P. Steyer, A.G. Sadowski, F. Beline, A waste characterisation procedure for ADM1 implementation based on degradation kinetics, Water Res. 46 (2012) 4099–4110.
[3] T. Lucas, D. Le Ray, P. Peu, M. Wagner, S. Picard, A new method for continuous assessment of CO2 released from dough baked in ventilated ovens, J. Food Eng. 81 (2007) 1–11.
[4] S. Picard, F. Beline, R. Girault, G. Bridoux, C. Cambert, A. Davenel, Determination of lipid fraction from organic wastes using Nuclear Magnetic Resonance (NMR): comparison to the soxhlet method. 13th World Congress on Anaerobic Digestion, Santiago de Compostela, Spain, 2014.
[5] Y. Bareha, R. Girault, J. Jimenez, A. Tremier, Characterization and prediction of organic nitrogen biodegradability during anaerobic digestion: a bioaccessibility approach, Bioresour. Technol. 263 (2018) 425–436.
[6] D.J. Batstone, J. Keller, I. Angelidaki, S.V. Kalyuzhnyi, S.G. Pavlostathis, A. Rozzi, W.T.M. Sanders, H. Siegrist, V.A. Vavilin, Anaerobic Digestion Model No.1 (ADM1), IWA Publishing, 2002.