ADM1F

0.1

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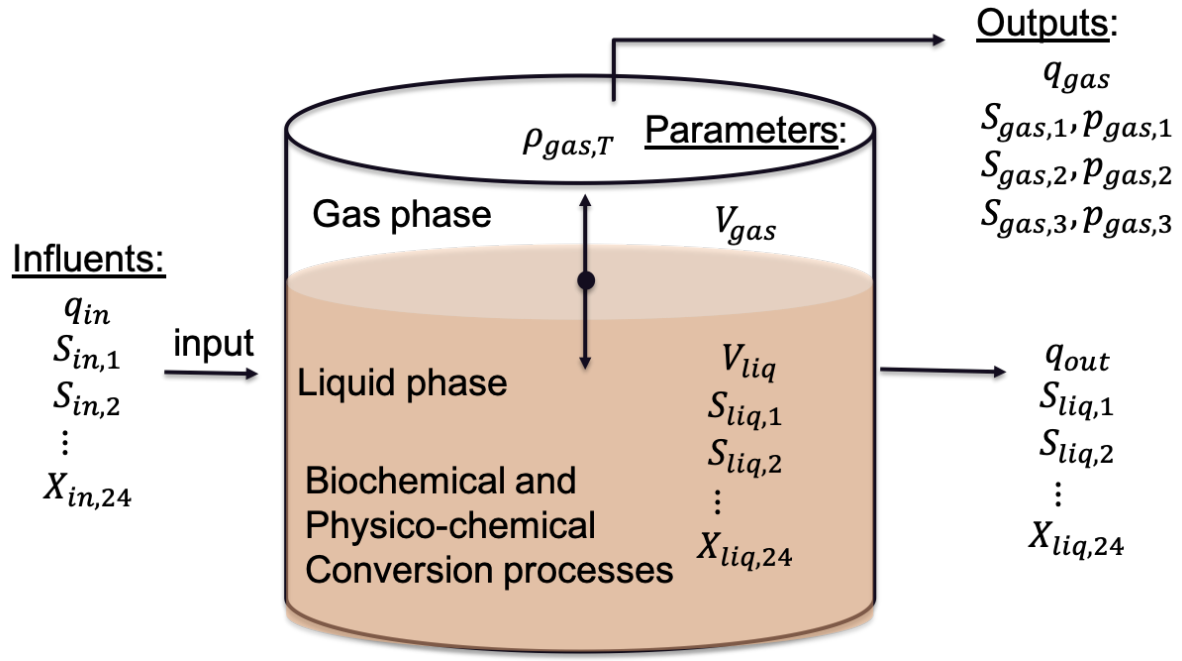
User Guide:

Anaerobic digestion (AD) process converts organic wastes into biogas. Biogas can generate heat and electricity through a cascade of biochemical reactions and has been adapted by various facilities and industries to treat and recover energy from high-strength liquid or solid waste streams. Anaerobic Digestion Model 1 (ADM1) is a mathematical model that describes the stoichiometry and kinetics of the essential biochemical reactions in AD. This repository includes C++ version of the Matlab/Simulink[1] version of the ADM1 model and the solid retention time (SRT) version[2]. The C++ version of the model is computationally more efficient than its Matlab/Simulink predecessor. We called this version of the model Anaerobic Digestion Model 1 Fast (ADM1F).



[1] Rosen C., Vrecko D., Gernaey K.V., Pons M.-N. and Jeppsson U. (2006). Implementing ADM1 for plant-wide benchmark simulations in Matlab/Simulink. Water Sci. Technol., 54(4), 11-19.

[2] *Zhu et al, in prep. A Novel Core-shell ADM1 model allows rapid optimization of membrane anaerobic digestion processes*

Chapter 1

Compile ADM1F

1. ADM1F uses external numerical library package PETSc. First download PETSc:

```
$ cd build; git clone -b release https://gitlab.com/petsc/petsc.git petsc
```

```
$ cd petsc; git checkout v3.14
```

2. Set **PETSC_DIR** and **PETSC_ARCH** in your environmental variables. We suggest to put these lines in your *~/.bashrc* or similar files (*~/.bash_profile* on Mac OS X). Once you add it into the bash file, run *source ~/.bash_profile*:

```
$ export PETSC_DIR=/path-to-my-ADM1F-folder/build/petsc
```

   and:

```
$ export PETSC_ARCH=macx-debug
```

   Make sure that 'adolc-utils' folder is in the 'build' folder.

3. Configure PETSC:

```
$ ./configure --download-mpich --with-cc=clang --with-fc=gfortran --with-debugging=0 --
↪download-adolc PETSC_ARCH=macx-debug --with-cxx-dialect=C++11 --download-colpack
```

NOTE: that these are for Mac OSX. If you are installing on a linux machine, then replace **clang** with **gcc**. Also, sometimes turning off *–with-fc=0* could help with compilation. This step will take awhile.

4. If configuration goes well, you can then compile. This step will take awhile too.:

```
$ make PETSC_DIR=/path-to-my-ADM1F-folder/build/petsc PETSC_ARCH=macx-debug all
```

5. After compilation, PETSc will show you how to test your installation (testing is optional).

6. Navigate back to the *build* folder (*cd ../*) and compile adm1f:

```
$ make adm1f
```

   or:

```
$ make
```

7. Set **ADM1F_EXE** in your environmental variable. Add this line in your *~/.bashrc* or similar files (*~/.bash_profile* on Mac OS X). Once you add it into the bash file, do not forget to *source ~/.bash_profile*:

```
$ export ADM1F_EXE=path-to-my-ADM1F-folder/build/adm1f
```

8. **NOTE**: There are two versions of the ADMF1: the original version (adm1f.cxx), and the modified version of the model (adm1f_srt.cxx, see *ADM1F SRT*).

Chapter 2

Running ADM1F

1. Make sure that **ADM1F_EXE:** is not empty (see step 7 from the previous section).:

```
$ echo $ADM1F_EXE
```

2. Navigate to the *simulations* folder and run the model:

```
$ $ADM1F_EXE

or using command-line options (see 4 and 5):

$ $ADM1F_EXE -ts_monitor -steady
```

3. Note that adm1f will look for three files *ic.dat*, *params.dat*, and *influent.dat*, which contain the initial conditions (45 values), parameters (100 values), and influent values (28 values), see *Inputs/Outputs*.
4. The command-line options are:
    - -Cat [val] - mass of Cat+ added [kmol/m3]
    - -Vliq [val] - volume of liquid [m3]
    - -Vgas [val] - volume of liquid [m3]
    - -t_resx [val] -SRT adjustment: t_resx = SRT-HRT, [d] (works only for adm1f_srt.cxx)
    - -params_file [filename] - specify params filename (default is params.dat)
    - -ic_file [filename] - specify initial conditions filename (default is ic.dat)
    - -influent_file [filename] - specify influent filename (default is influent.dat)
    - -ts_monitor - shows the timestep and time information on screen
    - -steady - run as steady state else runs as transient
    - -debug - gives out more details on the screen
5. More command-line options can be found here.

Chapter 3

ADM1F SRT

The adm1f_srt.cxx version includes solid retention time (SRT) and other modifications described below. To switch to the SRT version of the model change 'EXAMPLESC = adm1f_srt.cxx' , 'OBJECTS_PF = adm1f_srt.o', and 'adm1f: adm1f_srt.o' in the *build/makefile*. Then recompile the model (Compile ADM1F, step 6).

- Includes a term (T_resx) in the mass balance to separate the solids retention time from hydraulic retention time.
- Uses the empirical Hill function that describes the inhibition of acetogenesis and hydrogenotrophic methanogenesis by acetic acid with the noncompetitive inhibition model[1][2].
- Describes the inhibition of acetic acid on acetoclastic methanogenesis with the Haldane equation[3][4].
- Includes a adsorption-inhibition term describing the long-chain fatty acid[6] (LCFA) inhibition of LCFA degradation and methanogenesis.
- Includes Arrhenius equations describing the effect of temperature on bioreaction kinetics[5].
- Includes a cation term to simulate the addition of NaOH for pH adjustment.

References

[1] Love, N. G., R. J. Smith, K. R. Gilmore, and C. W. Randall. 1999. Oxime inhibition of nitrification during treatment of an ammonia-containing industrial waste. Water Environment Research 71:418–26.

[2] Oslislo, A., and Z. Lewandowski. 1985. Inhibition of nitrification in the packed bed reactors by selected organic compounds. Water Research 19:423–26.

[3] Haldane, J. B. S. 1930. Enzymes. London: Longmans.

[4] Andrews, J. F. 1968. A mathematical model for the continuous culture of microorganisms utilizing inhibitory substrates. Biotechnology and Bioengineering 10:707–23.

[6] Palatsi, J., Illa, J., Prenafeta-Boldú, F.X., Laureni, M., Fernandez, B., Angelidaki, I., Flotats. X. 2010. Long-chain fatty acids inhibition and adaptation process in anaerobic thermophilic digestion: Batch tests, microbial community structure and mathematical modelling. Bioresource Technology. 101, 7, 2243-2251.

[5] Novak, J. T. 1974. Temperature-substrate interactions in biological treatment. Journal, Water Pollution Control Federation 46:1984–94.

Chapter 4

Inputs/Outputs

4.1 Initial Conditions [ic.dat]

Index	Notation	Unit	Description
1	S_su	kgCOD/m3	soluble monosaccharides
2	S_aa	kgCOD/m3	soluble amino acids
3	S_fa	kgCOD/m3	soluble total LCFA
4	S_va	kgCOD/m3	soluble total valerate
5	S_bu	kgCOD/m3	soluble total butyrate
6	S_pro	kgCOD/m3	soluble total propionate
7	S_ac	kgCOD/m3	soluble acetate
8	S_h2	kgCOD/m3	hydrogen gas
9	S_ch4	kgCOD/m3	methane gas
10	S_IC	kmoleC/m3	soluble inorganic carbon
11	S_IN	kmoleC/m3	soluble inorganic nitrogen
12	S_I	kgCOD/m3	soluble inert materials
13	X_c_biom	kgCOD/m3	particulate of composites
14	X_ch_biom	kgCOD/m3	particulate of carbohydrate
15	X_pr_biom	kgCOD/m3	particulate of proteins
16	X_li_biom	kgCOD/m3	particulate of lipids
17	X_su	kgCOD/m3	monosaccharides degraders (microorganisms)
18	X_aa	kgCOD/m3	amino acids degraders (microorganisms)
19	X_fa	kgCOD/m3	LCFA degraders (microorganisms)
20	X_c4	kgCOD/m3	valerate and butyrate degraders (microorganisms)
21	X_pro	kgCOD/m3	propionate degraders (microorganisms)
22	X_ac	kgCOD/m3	acetate degraders (microorganisms)
23	X_h2	kgCOD/m3	hydrogen degraders (microorganisms)
24	X_I	kgCOD/m3	particulate of inerts
25	S_cation	kmole/m3	cations (strong base)
26	S_anion	kmole/m3	anions (strong acid)
27	S_hva	kgCOD/m3	soluble valerate acid
28	S_hbu	kgCOD/m3	soluble butyratic acid
29	S_hpro	kgCOD/m3	soluble propionatic acid
30	S_hac	kgCOD/m3	soluble acetatic acid
31	S_hco3	kmole/m3	soluble bicarbonate
32	S_nh3	kmole/m3	soluble ammonia
33	S_gas_h2	kgCOD/m3	soluble hydrogen gas
34	S_gas_ch4	kgCOD/m3	soluble methane gas

continues on next page

Table 1 – continued from previous page

Index	Notation	Unit	Description
35	S_gas_co2	kmole/m3	soluble carbon dioxide gas
36	Q	m3/d	flow rate
37	Temp	°C	temperature
38	S_D1_D	unitless	Dummy
39	S_D2_D	unitless	Dummy
40	S_D3_D	unitless	Dummy
41	X_D4_D	unitless	Dummy
42	X_D5_D	unitless	Dummy
43	S_H_ion	kmoleH+/m3	soluble hydrogen ion
44	S_co2	kmoleC/m3	soluble carbon dioxide
45	S_nh4	kmoleN/m3	soluble ammonium

4.2 Influent Data [influent.dat]

Index	Notation	Unit	Description
1	S_su_in	kgCOD/m3	soluble input monosaccharides
2	S_aa_in	kgCOD/m3	soluble input amino acids
3	S_fa_in	kgCOD/m3	soluble input total LCFA
4	S_va_in	kgCOD/m3	soluble input total valerate
5	S_bu_in	kgCOD/m3	soluble input total butyrate
6	S_pro_in	kgCOD/m3	soluble input total propionate
7	S_ac_in	kgCOD/m3	soluble input acetate
8	S_h2_in	kgCOD/m3	hydrogen gas
9	S_ch4_in	kgCOD/m3	methane gas
10	S_IC_in	kmoleC/m3	soluble input inorganic carbon
11	S_IN_in	kmoleC/m3	soluble input inorganic nitrogen
12	S_I_in	kgCOD/m3	soluble input inert materials
13	X_c_biom_in	kgCOD/m3	particulate input of composites
14	X_ch_biom_in	kgCOD/m3	particulate input of carbohydrate
15	X_pr_biom_in	kgCOD/m3	particulate input of proteins
16	X_li_biom_in	kgCOD/m3	particulate input of lipids
17	X_su_in	kgCOD/m3	monosaccharides degraders (microorganisms)
18	X_aa_in	kgCOD/m3	amino acids degraders (microorganisms)
19	X_fa_in	kgCOD/m3	LCFA degraders (microorganisms)
20	X_c4_in	kgCOD/m3	valerate and butyrate degraders (microorganisms)
21	X_pro_in	kgCOD/m3	propionate degraders (microorganisms)
22	X_ac_in	kgCOD/m3	acetate degraders (microorganisms)
23	X_h2_in	kgCOD/m3	hydrogen degraders (microorganisms)
24	X_I_in	kgCOD/m3	particulate input of inerts
25	S_cation_in	kmole/m3	input cations
26	S_anion_in	kmole/m3	input anions
27	Q	m3/d	flow rate
28	Temp	°C	temperature

4.3 Parameters [params.dat]

Index	Notation	Unit	Description
1	f_sI_xc	kgCOD/kg COD	fraction of composites (substrate) disintegrate to soluble inerts (product)
2	f_xI_xc	kgCOD/kg COD	fraction of composites (substrate) disintegrate to particulate inerts (product)
3	f_ch_xc	kgCOD/kg COD	fraction of composites (substrate) disintegrate to carbohydrates (product)
4	f_pr_xc	kgCOD/kg COD	fraction of composites (substrate) disintegrate to proteins (product)
5	f_li_xc	kgCOD/kg COD	fraction of composites (substrate) disintegrate to lipids (product)
6	N_xc	kmole N/(kg COD)	nitrogen content of composites
7	N_I	kmole N/(kg COD)	nitrogen content of inerts
8	N_aa	kmole N/(kg COD)	nitrogen content of amino acids
9	C_xc	kmole C/(kg COD)	carbon content of composites
10	C_sI	kmole C/(kg COD)	carbon content of soluble inerts
11	C_ch	kmole C/(kg COD)	carbon content of carbohydrates
12	C_pr	kmole C/(kg COD)	carbon content of proteins
13	C_li	kmole C/(kg COD)	carbon content of lipids
14	C_xI	kmole C/(kg COD)	carbon content of particulate inerts
15	C_su	kmole C/(kg COD)	carbon content of monosaccharides
16	C_aa	kmole C/(kg COD)	carbon content of amino acids
17	f_fa_li	kgCOD/kg COD	fraction of lipids (substrate) degrade to LCFA (product)
18	C_fa	kmole C/(kg COD)	carbon content of total LCFA
19	f_h2_su	kgCOD/kg COD	fraction of monosaccharides (substrate) degrade to hydrogen (product)
20	f_bu_su	kgCOD/kg COD	fraction of monosaccharides (substrate) degrade to butyrate (product)
21	f_pro_su	kgCOD/kg COD	fraction of monosaccharides (substrate) degrade to propionate (product)
22	f_ac_su	kgCOD/kg COD	fraction of monosaccharides (substrate) degrade to acetate (product)
23	N_bac	kmole N/(kg COD)	nitrogen content of synthesized into bacteria
24	C_bu	kmole C/(kg COD)	carbon content of total butyrate
25	C_pro	kmole C/(kg COD)	carbon content of total propionate
26	C_ac	kmole C/(kg COD)	carbon content of total acetate
27	C_bac	kmole C/(kg COD)	carbon content of synthesized into bacteria
28	Y_su	kgCOD_X/kg COD_S	yield of biomass on monosaccharides (substrate)
29	f_h2_aa	kgCOD/kg COD	fraction of amino acids (substrate) degrade to hydrogen (product)
30	f_va_aa	kgCOD/kg COD	fraction of amino acids (substrate) degrade to valerate (product)
31	f_bu_aa	kgCOD/kg COD	fraction of amino acids (substrate) degrade to butyrate (product)
32	f_pro_aa	kgCOD/kg COD	fraction of amino acids (substrate) degrade to propionate (product)
33	f_ac_aa	kgCOD/kg COD	fraction of amino acids (substrate) degrade to acetate (product)
34	C_va	kmole C/(kg COD)	carbon content of total valerate
35	Y_aa	kgCOD_X/kg COD_S	yield of biomass on amino acids (substrate)

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Table 2 – continued from previous page

Index	Notation	Unit	Description
36	Y_fa	kgCOD_X/kg COD_S	yield of biomass on total LCFA (substrate)
37	Y_c4	kgCOD_X/kg COD_S	yield of biomass on butyrate (substrate)
38	Y_pro	kgCOD_X/kg COD_S	yield of biomass on total propionate (substrate)
39	C_ch4	kmole C/(kg COD)	carbon content of methane
40	Y_ac	kgCOD_X/kg COD_S	yield of biomass on total acetate (substrate)
41	Y_h2	kgCOD_X/kg COD_S	yield of biomass on hydrogen (substrate)
42	k_dis	1/d	disintegration rate
43	k_hyd_ch	1/d	hydrolysis rate of carbohydrates (carbs to simple sugars)
44	k_hyd_pr	1/d	hydrolysis rate of proteins
45	k_hyd_li	1/d	hydrolysis rate of lipids
46	K_S_IN	kgCOD_S/m3	half saturation value of inorganic nitrogen
47	k_m_su	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for monosaccharides
48	K_S_su	kgCOD_S/m3	half saturation value of monosaccharides
49	pH_UL_acidac	unitless	upper pH limit of acidic acetate
50	pH_LL_acidac	unitless	lower pH limit of acidic acetate
51	k_m_aa	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for amino acids
52	K_S_aa	kgCOD_S/m3	half saturation value of amino acids
53	k_m_fa	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for total LCFA
54	K_S_fa	kgCOD_S/m3	half saturation value of total LCFA
55	K_Ih2_fa	kgCOD/m3	inhibition constant LCFA (substrate) degradation by hydrogen (inhibitor)
56	k_m_c4	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for butyrate and valerate
57	K_S_c4	kgCOD_S/m3	half saturation value of butyrate
58	K_Ih2_c4	kgCOD/m3	inhibition constant for butyrate and valerate (substrate) degradation by hydrogen (inhibitor)
59	k_m_pro	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for total propionate
60	K_S_pro	kgCOD_S/m3	half saturation value of total propionate
61	K_Ih2_pro	kgCOD/m3	inhibition constant for propionate (substrate) degradation by hydrogen (inhibitor)
62	k_m_ac	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for total acetate
63	K_S_ac	kgCOD_S/m3	half saturation value of total acetate
64	K_I_nh3	kmol N/m3	inhibition constant by ammonia (inhibitor)
65	pH_UL_ac	unitless	upper pH limit for total acetate
66	pH_LL_ac	unitless	lower pH limit for total acetate
67	k_m_h2	kgCOD_S/kgCOD_X/d	Monod maximum specific uptake rate for hydrogen
68	K_S_h2	kgCOD_S/m3	half saturation value of hydrogen
69	pH_UL_h2	unitless	upper pH limit for hydrogen
70	pH_LL_h2	unitless	lower pH limit for hydrogen
71	k_dec_Xsu	1/d	first order decay rate for the monosaccharide degraders

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Table 2 – continued from previous page

Index	Notation	Unit	Description
72	k_dec_Xaa	1/d	first order decay rate for the amino acids degraders
73	k_dec_Xfa	1/d	first order decay rate for the LCFA degraders
74	k_dec_Xc4	1/d	first order decay rate for the butyrate and valerate
75	k_dec_Xpro	1/d	first order decay rate for the propionate degraders
76	k_dec_Xac	1/d	first order decay rate for the acetate degraders
77	k_dec_Xh2	1/d	first order decay rate for the hydrogen degraders
78	R	bar m3 kmole-1 K-1	gas law constant (8.314e-2)
79	T_base	°C	base temperature
80	T_op	°C	operating temperature
81	pK_w_base	unitless	pKa of water
82	pK_a_va_base	unitless	pKa of total valerate
83	pK_a_bu_base	unitless	pKa of total butyrate
84	pK_a_pro_base	unitless	pKa of total propionate
85	pK_a_ac_base	unitless	pKa of total acetate
86	pK_a_co2_base	unitless	pKa of carbon dioxide
87	pK_a_IN_base	unitless	pKa of inorganic nitrogen
88	pK_a_hco3_base	unitless	pKa of bicarbonate
89	k_A_Bbu	1/M/d	acid base kinetic parameter for total butyrate
90	k_A_Bpro	1/M/d	acid base kinetic parameter for total propionate
91	k_A_Bac	1/M/d	acid base kinetic parameter for total acetate
92	k_A_Bco2	1/M/d	acid base kinetic parameter for carbon dioxide
93	k_A_BIN	1/M/d	acid base kinetic parameter for inhibitors
94	P_atm	bar	atmospheric pressure
95	kLa	1/d	gas-liquid transfer coefficient
96	K_H_h2o_base	M(liq)/bar	Henry's law coefficient of water
97	K_H_co2_base	M(liq)/bar	Henry's law coefficient of carbon dioxide
98	K_H_ch4_base	M(liq)/bar	Henry's law coefficient of methane
99	K_H_h2_base	M(liq)/bar	Henry's law coefficient of hydrogen
100	k_P	m2/d/bar	proportional gain

4.4 Outputs [indicator***.out]

Index	Notation	Unit	Description
1	Ssu	mg COD/L	soluble monosaccharides
2	Saa	mg COD/L	soluble amino acids
3	Sfa	mg COD/L	soluble total LCFA
4	Sva	mg COD/L	soluble total valerate
5	Sbu	mg COD/L	soluble total butyrate
6	Spro	mg COD/L	soluble total propionate
7	Sac	mg COD/L	soluble total acetate
8	Sh2	mg COD/L	soluble hydrogen
9	Sch4	mg COD/L	soluble methane
10	Sic	mg C/L	soluble inorganic carbon
11	Sin	mg N/L	soluble inorganic nitrogen
12	Si	mg COD/L	soluble inerts
13	Xc	mg COD/L	particulate composites
14	Xch	mg COD/L	particulate carbohydrates
15	Xpr	mg COD/L	particulate proteins
16	Xli	mg COD/L	particulate lipids
17	Xsu	mg COD/L	monosaccharides degraders (microorganisms)

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Table 3 – continued from previous page

Index	Notation	Unit	Description
18	Xaa	mg COD/L	amino acids degraders (microorganisms)
19	Xfa	mg COD/L	LCFA degraders (microorganisms)
20	Xc4	mg COD/L	butyrate and valerate degraders (microorganisms)
21	Xpro	mg COD/L	propionate degraders (microorganisms)
22	Xac	mg COD/L	acetate degraders (microorganisms)
23	Xh2	mg COD/L	hydrogen degraders (microorganisms)
24	Xi	mg COD/L	particulate inerts
25	scat+	mmol/L	cations
26	san-	mmol/L	anions
27	pH	unitless	a scale used to specify how acidic or basic a water-based solution is
28	S_H+	mol/L	soluble hydrogen cation
29	Sva-	mg COD/L	soluble total valerate anion
30	Sbu-	mg COD/L	soluble total butyrate anion
31	Spro-	mg COD/L	soluble total propionate anion
32	Sac-	mg COD/L	soluble total acetate anion
33	Shco3-	mmol C/L	soluble bicarbonate anion
34	Sco2	mmol C/L	soluble carbon dioxide
35	Snh3	mg N/L	soluble ammonia
36	Snh4+	mg N/L	soluble ammonia cation (ammonium)
37	Sgas,h2	mg COD/L	soluble hydrogen gas
38	Sgas,ch4	mg COD/L	soluble methane gas
39	Sgas,co2	mmol C/L	soluble carbon dioxide gas
40	pgas,h2	atm	partial pressure of gas hydrogen
41	pgas,ch4	atm	partial pressure of gas methane
42	pgas,co2	atm	partial pressure of gas carbon dioxide
43	pgas,total	atm	partial pressure of gas all gases
44	pgas	m3/d	flow rate of gas
45	Si	mg COD/L	soluble inert organics
46	Ss	mg COD/L	readily biodegradable substrate
47	Xi	mg COD/L	particulate inert organics
48	Xs	mg COD/L	slowly biodegradable substrate
49	Xd	mg COD/L	particulate arising from biomass decay decay
50	Snh	mg N/L	ammonia and ammonium nitrogen, soluble the ammonia produced during ammonification process from soluble organic nitrogen
51	Sns	mg N/L	soluble biodegradable organic nitrogen generated during hydrolysis of particulate biodegradable organic nitrogen, suggesting it is the concentration of soluble organic hydrogen generated during hydrolysis
52	Xns	mg N/L	particulate biodegradable organic nitrogen generated during hydrolysis of particulate biodegradable organic nitrogen, suggesting it is the concentration of soluble organic hydrogen generated during hydrolysis
53	Salk	mg C/L	charge balance
54	TSS	mg TSS/L	total suspended solids
55	VFA_C2toC5	mg COD/L	volatile fatty acid from C2 to C5
56	mass_Sac	mg Hac/L	acetic acid
57	PAratio	kg acetate/ kg acetate equivalent of propionate	acetate propionate ratio

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Table 3 – continued from previous page

Index	Notation	Unit	Description
58	Alk	mg/L CaCO3	alkalinity
59	NH3	mg N/L	ammonia
60	NH4	mg N/L	ammonium
61	LCFA	mgCOD_LCFA/L	long chain fatty acid
62	percentch4	%	biogas methane content, methane percentage output, percent by volume
63	energych4	%	energy content of CH4 gas, methane energy output, methane converted to COD, percentage of input that's converted to CH4 energy wise
64	efficiency	%	COD removal
65	VFA/ALK	g acetate eq./g CaCO3	volatile fatty acid to alkalinity ratio
66	ACN	kg COD/m3/d	acetate capacity number, the ratio between the maximum acetate utilization rate and the average acetate production rate
67	SampleT	d	

examples # join

References

Acknowledgements

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