Real-Time Substrate Feed Optimization of Anaerobic Co-Digestion Plants

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Appendix A

Anaerobic Digestion Model (Simple)

In the following the anaerobic digestion model, used in Section 4.4 to compare different state estimation schemes, is presented. It is the implementation used in Shen et al. (2006). The state equations are given in equation (A.1). The state, output and input variables are explained in Table 4.1 and all model parameters in Table A.1.

$$\begin{aligned}
S'(t) &= D \cdot (S_i(t) - S(t)) - f_a\left(S(t), S_i(t)\right) \cdot X_a(t) \cdot Y_a \\
X'_a(t) &= \left[f_a\left(S(t), S_i(t)\right) - D_a\right] \cdot X_a(t) \\
V'_a(t) &= -D \cdot V_a(t) + f_a\left(S(t), S_i(t)\right) \cdot X_a(t) \cdot y^{\mathrm{a}}_{\mathrm{vf}} - \\
&\quad - f_m\left(\left(H_a \circ V_a\right)(t)\right) \cdot X_m(t) \cdot Y_m \\
X'_m(t) &= \left[f_m\left(\left(H_a \circ V_a\right)(t)\right) - D_m\right] \cdot X_m(t) \\
C'(t) &= -D \cdot C(t) + f_a\left(S(t), S_i(t)\right) \cdot X_a(t) \cdot y^{\mathrm{a}}_{\mathrm{co_2}} + \\
&\quad + f_m\left(\left(H_a \circ V_a\right)(t)\right) \cdot X_m(t) \cdot y^{\mathrm{m}}_{\mathrm{co_2}} - k_{\mathrm{la}} \cdot \left(C(t) - k_{\mathrm{h}} \cdot P_c(t)\right) \\
P'_c(t) &= k_{\mathrm{g}} \cdot \left[k_{\mathrm{la}} \cdot \left(1 - P_c(t)\right) \cdot \left(C(t) - k_{\mathrm{h}} \cdot P_c(t)\right) - \right. \\
&\quad \left. - r_{\mathrm{g}} \cdot P_c(t) \cdot f_m\left(\left(H_a \circ V_a\right)(t)\right) \cdot X_m(t) \cdot y^{\mathrm{m}}_{\mathrm{ch_4}}\right]
\end{aligned} \tag{A.1}$$

The model outputs are produced methane $Q_{\mathrm{ch_4}}$ and carbon dioxide $Q_{\mathrm{co_2}}$ as well as the pH value of the reactor. The output equations are given in eq. (A.2).

$$\begin{aligned}
Q_{\mathrm{ch_4}}(t) &= k_{\mathrm{g}} \cdot r_{\mathrm{g}} \cdot f_m\left(\left(H_a \circ V_a\right)(t)\right) \cdot X_m(t) \cdot y^{\mathrm{m}}_{\mathrm{ch_4}} \\
Q_{\mathrm{co_2}}(t) &= k_{\mathrm{g}} \cdot k_{\mathrm{la}} \cdot \left(C(t) - k_{\mathrm{h}} \cdot P_c(t)\right) \\
\mathrm{pH}(t) &= -\log_{10}\left(c\left(\mathrm{H}^+(t)\right)\right)
\end{aligned} \tag{A.2}$$

Further variables of the model are given in equation (A.3).

$$\begin{aligned}
Y_a &:= y^{\mathrm{a}}_{\mathrm{vf}} + y^{\mathrm{a}}_{\mathrm{co_2}} + \frac{1}{y^{\mathrm{a}}_{\mathrm{s}}} & \qquad Y_m &:= y^{\mathrm{m}}_{\mathrm{ch_4}} + y^{\mathrm{m}}_{\mathrm{co_2}} + \frac{1}{y^{\mathrm{m}}_{\mathrm{s}}} \\
D_a &:= \chi \cdot D + k_{\mathrm{da}} & \qquad D_m &:= \chi \cdot D + k_{\mathrm{dm}} \\
k_{\mathrm{g}} &:= \frac{S_{\mathrm{v}} \cdot V_{\mathrm{liq}}}{C_{\mathrm{co_2}} \cdot V_{\mathrm{gas}}} & \qquad r_{\mathrm{g}} &:= \frac{C_{\mathrm{co_2}}}{C_{\mathrm{ch4}}}
\end{aligned} \tag{A.3}$$

The growth rate of the acidogenic bacterial population is modeled by f_a and the one for the methanogenic population by f_m, both are given in equation (A.4).

$$\begin{aligned} f_a\left(S(t), S_i(t)\right) &= \frac{\mu_{\max}^{\mathrm{a}} \cdot S(t)}{k_{\mathrm{sa}} + S(t)} \cdot \frac{k_{\mathrm{sa}} + S_i(t)}{S_i(t)} \\ f_m\left(\left(H_a \circ V_a\right)(t)\right) &= \frac{\mu_{\max}^{\mathrm{m}} \cdot \left(H_a \circ V_a\right)(t)}{\left(H_a \circ V_a\right)(t) + k_{\mathrm{sm}} + \frac{\left(\left(H_a \circ V_a\right)(t)\right)^2}{k_{\mathrm{im}}}} \end{aligned} \tag{A.4}$$

The undissociated fraction of the acetic acid concentration V_a is symbolized by H_a and given in equation (A.5). The needed hydrogen cation concentration $c\left(\mathrm{H}^+(t)\right)$ is governed by the cubic equation in (A.6).

$$H_a\left(V_a(t)\right) := \left(H_a \circ V_a\right)(t) := \frac{V_a(t) \cdot c\left(\mathrm{H}^+(t)\right)}{k_{\mathrm{a}} + c\left(\mathrm{H}^+(t)\right)} \tag{A.5}$$

$$\begin{aligned} \left(c\left(\mathrm{H}^+(t)\right)\right)^3 + \left(k_{\mathrm{a}} + B_{ic}(t)\right) \cdot \left(c\left(\mathrm{H}^+(t)\right)\right)^2 - \\ - \left[k_{\mathrm{a}} \cdot \left(V_a(t) - B_{ic}(t)\right) + k_{\mathrm{w}} + k_{\mathrm{h}} \cdot k_{\mathrm{co_2}} \cdot P_c(t)\right] \cdot c\left(\mathrm{H}^+(t)\right) = \\ = k_{\mathrm{a}} \cdot \left(k_{\mathrm{w}} + k_{\mathrm{h}} \cdot k_{\mathrm{co_2}} \cdot P_c(t)\right) \end{aligned} \tag{A.6}$$

Table A.1: Model parameters as in Shen et al. (2006).

Parameter	Value	Unit	Description
$\mu^{\mathrm{a}}_{\mathrm{max}}$	0.5033	h^{-1}	Maximum growth rate of acidogenic bacteria
k_{sa}	238.1	mg/l	Acidogenic bacteria half-velocity
k_{da}	$3.1e^{-2}$	h^{-1}	Acidogenic bacteria decay rate
$\mu^{\mathrm{m}}_{\mathrm{max}}$	$2.27e^{-3}$	h^{-1}	Maximum growth rate of methanogenic bacteria
k_{sm}	$1.45e^{-2}$	mg/l	Methanogenic bacteria half-velocity
k_{im}	35.47	mg/l	Methanogenic bacteria inhibtion concentration
k_{dm}	$8e^{-4}$	h^{-1}	Methanogenic bacteria decay rate
$y^{\mathrm{a}}_{\mathrm{s}}$	0.688	–	Yield coefficient (substrate to acidogenic bacteria)
$y^{\mathrm{a}}_{\mathrm{vf}}$	0.6427	–	Yield coefficient (substrate to acetic acid)
$y^{\mathrm{a}}_{\mathrm{co_2}}$	0.5	–	Yield coefficient (substrate to CO_2)
$y^{\mathrm{m}}_{\mathrm{s}}$	3.27	–	Yield coefficient (acetic acid to methanogenic bacteria)
$y^{\mathrm{m}}_{\mathrm{ch_4}}$	20.732	–	Yield coefficient (acetic acid to CH_4)
$y^{\mathrm{m}}_{\mathrm{co_2}}$	5.174	–	Yield coefficient (acetic acid to CO_2)
k_{w}	$1e^{-14}$	–	Water dissociation constant
$k_{\mathrm{co_2}}$	$4.5e^{-7}$	–	Carbonic acid dissociation constant
k_{h}	$1.08e^{3}$	–	Henry's law constant
k_{a}	$1.85e^{-5}$	–	Weak acid dissociation constant
k_{la}	6.832	–	CO_2 mass transfer rate coefficient
S_{v}	22.4	–	Avogadro's constant
$C_{\mathrm{co_2}}$	$4.4e4$	–	mole to mg/l conversion constant for CO_2
C_{ch4}	$1.6e4$	–	mole to mg/l conversion constant for CH_4
χ	0.01667	–	Liquid/solid dilution rate ratio
D	0.042	h^{-1}	Dilution rate
V_{liq}	30	l	Liquid phase volume
V_{gas}	5	l	Gas phase volume
P_t	1	atm	Total pressure in the gas phase

Appendix B

Biogas Toolbox in MATLAB®

In this thesis detailed simulation models of biogas plants play a key role. In MATLAB®, more precisely in Simulink®, simulation models can be created quite easily. Therefore, MATLAB® was used as a platform to develop a general model for biogas plants, as well as all other components developed in this thesis, such as the state estimators and the NMPC.

The key idea of the developed MATLAB® toolbox is to treat algorithms for optimization and control and biogas simulation models separately. The advantage is that all algorithms can be easily applied to different tasks and different biogas plant models as well. The result is a collection of 16 different MATLAB® toolboxes, each with its own purpose. Seven of these toolboxes have something to do with biogas and three toolboxes form the foundation of each of the other toolboxes and have no own use. The remaining six toolboxes have each their special purpose and can be used independently of the others. Their purposes for example are data analysis, file-I/O, machine learning or optimization. The following list gives an overview.

- biogas_blocks: Simulink® blocks to create complex models of biogas plants.
- biogas_calibration: Framework to automatically calibrate the ADM1 parameters of a biogas plant model.
- biogas_control: Contains the algorithms of the NMPC for optimal feed control of biogas plants.
- biogas_gui: GUIs to create and define the simulation model, feeds, boundaries, etc.
- biogas_ml: Framework to use machine learning methods in biogas applications.
- biogas_optimization: Framework to use optimization methods in biogas applications.
- biogas_scripts: Collection of useful functions in biogas applications.
- data_tool: Collection of functions for data preparation and visualization.
- doc_tool: Creates the online documentation of all functions in the other tool-

boxes.

- gecoc_tool_def: Needed for all toolboxes.
- io_tool: Collection of functions for file-I/O.
- ml_tool: Collection of functions that belong to the family of machine learning.
- numerics_tool: Contains classes and functions to perform some numerical mathematics.
- optimization_tool: Collection of optimization methods.
- script_collection: Collection of functions that are generally useful.
- setup_tool: Provides a general installation method that is used by all other toolboxes.

The separation of methods and models requires general algorithms and methods, but also the models must somehow be general. As prerequisite all models have to be designed following the same guidelines, which are facilitated by using well-developed graphical user interfaces (GUIs) implemented in the toolbox. With these GUIs the user can e.g. specify the setup of the plant, like the number and properties of the fermenters as well as those for the cogeneration units available on the plant. Furthermore, physical and chemical characteristics of the substrate feed can be specified (see Figure B.1), which makes detailed simulations of various substrate mixtures possible. The toolbox then uses this information to semi-automatically generate a Simulink® model of the specified biogas plant, which by default satisfies the needed guidelines (see Figure 7.6). This developed model then can be used to learn the state estimator in Chapter 8 or as prediction model inside the control application in Chapter 9.

To improve the speed of the simulations parts of the algorithms are implemented in C#. The implemented classes are included in MATLAB® by importing them as DLLs. Upon request the complete MATLAB® toolbox is given to the interested user licensed under the GNU General Public Licence[1].

[1] `http://www.gnu.org/copyleft/gpl.html`

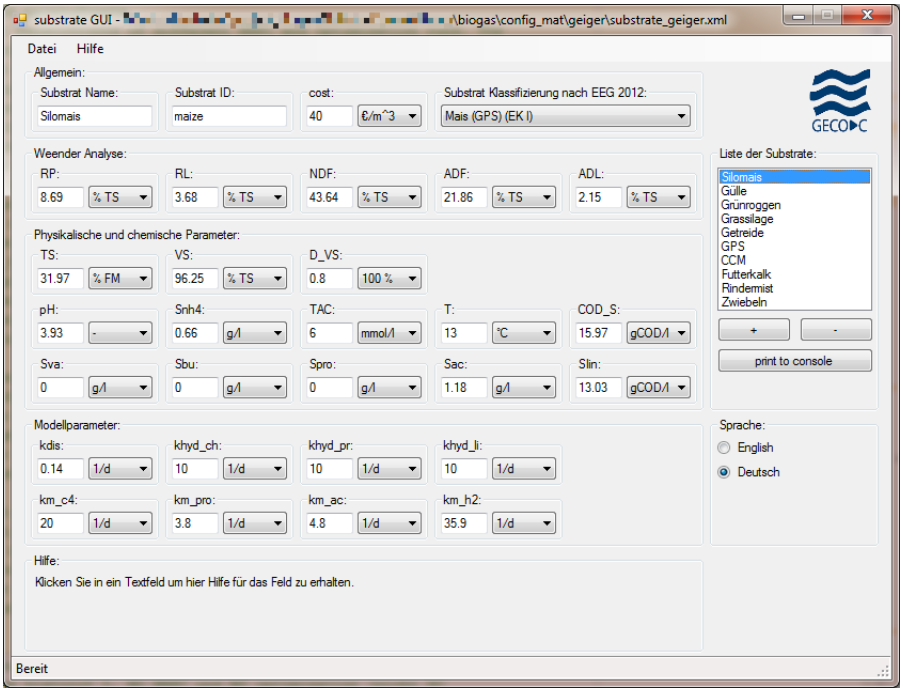

Figure B.1: GUI to define chemical and physical parameters of the substrate feed.

Appendix C

ADM1: Petersen Matrix and Model Parameters

On the following pages the parameters and variables of the ADM1, introduced in Section 7.1, are given. The ADM1 is modeled as a system of ordinary differential equations. The system equation is given in eq. (7.1) and is repeated here for convenience.

$$ {}^{o}\boldsymbol{x}_{\mathrm{AD}}{}'(\tau) = \boldsymbol{D}_u(\tau) \cdot {}^{o}\boldsymbol{u}_{\mathrm{AD}}(\tau) - \boldsymbol{D}_x(\tau) \cdot {}^{o}\boldsymbol{x}_{\mathrm{AD}}(\tau) + \boldsymbol{V} \left({}^{o}\boldsymbol{x}_{\mathrm{AD}}\right)^T \cdot \boldsymbol{\rho} \left({}^{o}\boldsymbol{x}_{\mathrm{AD}}\right) \tag{C.1} $$

The input $\boldsymbol{D}_u$ and state transition matrix $\boldsymbol{D}_x$ are given in eq. (C.2). There, $\mathbf{1}_{33} \in \mathbb{N}_0^{33\times 33}$ is the 33 dimensional identity matrix and $\mathbf{0}_{n\times m}$ is the $n \times m$ dimensional zero matrix, $n, m \in \mathbb{N}_0$.

$$ \begin{aligned} \boldsymbol{D}_u(\tau) &:= \begin{pmatrix} D(\tau)\cdot \mathbf{1}_{33} & \mathbf{0}_{33\times 1} \\ \mathbf{0}_{4\times 33} & \mathbf{0}_{4\times 1} \end{pmatrix} \in \mathbb{R}^{37\times 34} \qquad D(\tau) := \frac{{}^{o}u_{\mathrm{AD},34}(\tau)}{V_{\mathrm{liq}}} \overset{(7.2)}{=} \frac{Q_{\mathrm{IN}}}{V_{\mathrm{liq}}} \\ \boldsymbol{D}_x(\tau) &:= \begin{pmatrix} D(\tau)\cdot \mathbf{1}_{33} & \mathbf{0}_{33\times 4} \\ \mathbf{0}_{4\times 33} & \mathbf{0}_{4\times 4} \end{pmatrix} \in \mathbb{R}^{37\times 37} \end{aligned} \tag{C.2} $$

The stoichiometric matrix $\boldsymbol{V} : \mathbb{R}^{37} \to \mathbb{R}^{29\times 37}$ and the vector of process rates $\boldsymbol{\rho} : \mathbb{R}^{37} \to \mathbb{R}^{29}$ are given in the Petersen matrix (Henze et al., 2000) form, see Tables C.1 and C.2. The matrix layout is $[\boldsymbol{V} \,|\boldsymbol{\rho}]$. The process rate vector $\boldsymbol{\rho}$ is shown in eq. (C.3). All variables and parameters of the ADM1 are given in eqs. (C.4) - (C.6) and Table C.3, respectively. The implementation and all values are adapted from Tschepetzki and Ogurek (2010).

Table C.1: ADM1 Petersen Matrix: Part I

	Component →	i	1	2	3	4	5	6	7	8	9	10	11	12	13	14
j	Process ↓		S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	S_{co2}	S^{+}_{nh4}	S_{I}	X_{c}	X_{ch}
1	Disintegration											$f_{co2,Xc}$		$f_{si,Xc}$	-1	$f_{ch,Xc}$
2	Hydrolysis of X_{ch}		1													-1
3	Hydrolysis of X_{pr}			1												
4	Hydrolysis of lipids		$1-f_{fa,li}$		$f_{fa,li}$							$f_{co2,Xli}$				
5	Uptake of sugars		-1				$(1-Y_{su})\cdot f_{bu,su}$	$(1-Y_{su})\cdot f_{pro,su}$	$(1-Y_{su})\cdot f_{ac,su}$	$(1-Y_{su})\cdot f_{h2,su}$		$f_{co2,su}$	$-Y_{su}\cdot N_{xb}$			
6	Uptake of S_{aa}			-1		$(1-Y_{aa})\cdot f_{va,aa}$	$(1-Y_{aa})\cdot f_{bu,aa}$	$(1-Y_{aa})\cdot f_{pro,aa}$	$(1-Y_{aa})\cdot f_{ac,aa}$	$(1-Y_{aa})\cdot f_{h2,aa}$		$f_{co2,aa}$	$N_{aa}-Y_{aa}\cdot N_{xb}$			
7	Uptake of LCFA				-1				$(1-Y_{fa})\cdot f_{ac,fa}$	$(1-Y_{fa})\cdot f_{h2,fa}$		$f_{co2,fa}$	$-Y_{fa}\cdot N_{xb}$			
8	Uptake of valerate					-1		$(1-Y_{c4})\cdot f_{pro,va}$	$(1-Y_{c4})\cdot f_{ac,va}$	$(1-Y_{c4})\cdot f_{h2,va}$		$f_{co2,va}$	$-Y_{c4}\cdot N_{xb}$			
9	Uptake of butyrate						-1		$(1-Y_{c4})\cdot f_{ac,bu}$	$(1-Y_{c4})\cdot f_{h2,bu}$		$f_{co2,bu}$	$-Y_{c4}\cdot N_{xb}$			
10	Uptake of propionate							-1	$(1-Y_{pro})\cdot f_{ac,pro}$	$(1-Y_{pro})\cdot f_{h2,pro}$		$f_{co2,pro}$	$-Y_{pro}\cdot N_{xb}$			
11	Uptake of acetate								-1		$1-Y_{ac}$	$f_{co2,ac}$	$-Y_{ac}\cdot N_{xb}$			
12	Uptake of hydrogen									-1	$1-Y_{h2}$	$f_{co2,h2}$	$-Y_{h2}\cdot N_{xb}$			
13	Decay of X_{su}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
14	Decay of X_{aa}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
15	Decay of X_{fa}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
16	Decay of X_{c4}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
17	Decay of X_{pro}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
18	Decay of X_{ac}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
19	Decay of X_{h2}											$f_{co2,xb}$	$f_{sin,xb}$			$f_{ch,xb}$
20	S_{hva}/S^{-}_{va} equil.															
21	S_{hbu}/S^{-}_{bu} equil.															
22	S_{hpro}/S^{-}_{pro} equil.															
23	S_{hac}/S^{-}_{ac} equil.															
24	S_{co2}/S^{-}_{hco3} equil.											1				
25	S^{+}_{nh4}/S_{nh3} equil.												1			
26	part. pressure S_{h2}									$-\frac{V_{gas}}{V_{liq}}$						
27	part. pressure S_{ch4}										$-\frac{V_{gas}}{V_{liq}}$					
28	part. pressure S_{co2}											$-\frac{V_{gas}}{V_{liq}}$				
29	total part. pressure															

Table C.2: ADM1 Petersen Matrix: Part II

	Component →	i	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	process rate
j	Process ↓		X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	X_{I}	X_{p}	S_{cat}^{+}	S_{an}^{-}	S_{va}^{-}	S_{bu}^{-}	S_{pro}^{-}	S_{ac}^{-}	S_{hco3}^{-}	S_{nh3}	pi_{Sh2}	pi_{Sch4}	pi_{Sco2}	p_{total}	ρ_j
1	Disintegration		$f_{pr,Xc}$	$f_{li,Xc}$								$f_{xi,Xc}$	$f_{xp,Xc}$													ρ_1
2	Hydrolysis of X_{ch}																									ρ_2
3	Hydrolysis of X_{pr}		-1																							ρ_3
4	Hydrolysis of lipids			-1																						ρ_4
5	Uptake of sugars				Y_{su}																					ρ_5
6	Uptake of S_{aa}					Y_{aa}																				ρ_6
7	Uptake of LCFA						Y_{fa}																			ρ_7
8	Uptake of valerate							Y_{c4}																		ρ_8
9	Uptake of butyrate							Y_{c4}																		ρ_9
10	Uptake of propionate								Y_{pro}																	ρ_{10}
11	Uptake of acetate									Y_{ac}																ρ_{11}
12	Uptake of hydrogen										Y_{h2}															ρ_{12}
13	Decay of X_{su}		$f_{pr,xb}$	$f_{li,xb}$	-1								f_{p}													ρ_{13}
14	Decay of X_{aa}		$f_{pr,xb}$	$f_{li,xb}$		-1							f_{p}													ρ_{14}
15	Decay of X_{fa}		$f_{pr,xb}$	$f_{li,xb}$			-1						f_{p}													ρ_{15}
16	Decay of X_{c4}		$f_{pr,xb}$	$f_{li,xb}$				-1					f_{p}													ρ_{16}
17	Decay of X_{pro}		$f_{pr,xb}$	$f_{li,xb}$					-1				f_{p}													ρ_{17}
18	Decay of X_{ac}		$f_{pr,xb}$	$f_{li,xb}$						-1			f_{p}													ρ_{18}
19	Decay of X_{h2}		$f_{pr,xb}$	$f_{li,xb}$							-1		f_{p}													ρ_{19}
20	S_{hva}/S_{va}^{-} equil.															-1										ρ_{20}
21	S_{hbu}/S_{bu}^{-} equil.																-1									ρ_{21}
22	S_{hpro}/S_{pro}^{-} equil.																	-1								ρ_{22}
23	S_{hac}/S_{ac}^{-} equil.																		-1							ρ_{23}
24	S_{co2}/S_{hco3}^{-} equil.																			-1						ρ_{24}
25	S_{nh4}^{+}/S_{nh3} equil.																				-1					ρ_{25}
26	part. pressure S_{h2}																					$\frac{R\cdot T}{16}$			$\frac{R\cdot T}{16}$	ρ_{26}
27	part. pressure S_{ch4}																						$\frac{R\cdot T}{64}$		$\frac{R\cdot T}{64}$	ρ_{27}
28	part. pressure S_{co2}																							$R\cdot T$	$R\cdot T$	ρ_{28}
29	total part. pressure																					$-\frac{pi_{Sh2}}{p_{total}}$	$-\frac{pi_{Sch4}}{p_{total}}$	$-\frac{pi_{Sco2}}{p_{total}}$	-1	ρ_{29}

Process rate vector $\boldsymbol{\rho}$:

$$\boldsymbol{\rho} := \begin{pmatrix} k_{\mathrm{dis}} \cdot X_{\mathrm{c}} \\ k_{\mathrm{hyd,ch}} \cdot X_{\mathrm{ch}} \cdot \frac{1}{1+\left(\frac{\mathrm{TS}}{K_{\mathrm{hyd}}}\right)^{n_{\mathrm{hyd}}}} \\ k_{\mathrm{hyd,pr}} \cdot X_{\mathrm{pr}} \cdot \frac{1}{1+\left(\frac{\mathrm{TS}}{K_{\mathrm{hyd}}}\right)^{n_{\mathrm{hyd}}}} \\ k_{\mathrm{hyd,li}} \cdot X_{\mathrm{li}} \cdot \frac{1}{1+\left(\frac{\mathrm{TS}}{K_{\mathrm{hyd}}}\right)^{n_{\mathrm{hyd}}}} \\ \frac{k_{\mathrm{m,su}} \cdot S_{\mathrm{su}}}{K_{\mathrm{S,su}}+S_{\mathrm{su}}} \cdot X_{\mathrm{su}} \cdot I_1 \\ \frac{k_{\mathrm{m,aa}} \cdot S_{\mathrm{aa}}}{K_{\mathrm{S,aa}}+S_{\mathrm{aa}}} \cdot X_{\mathrm{aa}} \cdot I_1 \\ \frac{k_{\mathrm{m,fa}} \cdot S_{\mathrm{fa}}}{K_{\mathrm{S,fa}}+S_{\mathrm{fa}}} \cdot X_{\mathrm{fa}} \cdot I_1 \cdot I_{\mathrm{H2,fa}} \\ \frac{k_{\mathrm{m,c4}} \cdot S_{\mathrm{va}}}{K_{\mathrm{S,c4}}+S_{\mathrm{va}}} \cdot X_{\mathrm{c4}} \cdot \frac{S_{\mathrm{va}}}{S_{\mathrm{va}}+S_{\mathrm{bu}}} \cdot I_1 \cdot I_{\mathrm{H2,c4}} \\ \frac{k_{\mathrm{m,c4}} \cdot S_{\mathrm{bu}}}{K_{\mathrm{S,c4}}+S_{\mathrm{bu}}} \cdot X_{\mathrm{c4}} \cdot \frac{S_{\mathrm{bu}}}{S_{\mathrm{va}}+S_{\mathrm{bu}}} \cdot I_1 \cdot I_{\mathrm{H2,c4}} \\ \frac{k_{\mathrm{m,pro}} \cdot S_{\mathrm{pro}}}{K_{\mathrm{S,pro}}+S_{\mathrm{pro}}} \cdot X_{\mathrm{pro}} \cdot I_1 \cdot I_{\mathrm{H2,pro}} \\ \frac{k_{\mathrm{m,ac}} \cdot S_{\mathrm{ac}}}{K_{\mathrm{S,ac}}+S_{\mathrm{ac}}} \cdot X_{\mathrm{ac}} \cdot I_{\mathrm{in}} \cdot I_{\mathrm{NH3}} \cdot I_{\mathrm{pH,ac}} \\ \frac{k_{\mathrm{m,h2}} \cdot S_{\mathrm{h2}}}{K_{\mathrm{S,h2}}+S_{\mathrm{h2}}} \cdot X_{\mathrm{h2}} \cdot I_{\mathrm{in}} \cdot I_{\mathrm{pH,h2}} \\ k_{\mathrm{dec,su}} \cdot X_{\mathrm{su}} \\ k_{\mathrm{dec,aa}} \cdot X_{\mathrm{aa}} \\ k_{\mathrm{dec,fa}} \cdot X_{\mathrm{fa}} \\ k_{\mathrm{dec,c4}} \cdot X_{\mathrm{c4}} \\ k_{\mathrm{dec,pro}} \cdot X_{\mathrm{pro}} \\ k_{\mathrm{dec,ac}} \cdot X_{\mathrm{ac}} \\ k_{\mathrm{dec,h2}} \cdot X_{\mathrm{h2}} \\ k_{\mathrm{A/Bva}} \cdot \left(S_{\mathrm{va}}^{-} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,va}} \cdot S_{\mathrm{hva}}\right) \\ k_{\mathrm{A/Bbu}} \cdot \left(S_{\mathrm{bu}}^{-} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,bu}} \cdot S_{\mathrm{hbu}}\right) \\ k_{\mathrm{A/Bpro}} \cdot \left(S_{\mathrm{pro}}^{-} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,pro}} \cdot S_{\mathrm{hpro}}\right) \\ k_{\mathrm{A/Bac}} \cdot \left(S_{\mathrm{ac}}^{-} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,ac}} \cdot S_{\mathrm{hac}}\right) \\ k_{\mathrm{A/Bco2}} \cdot \left(S_{\mathrm{hco3}}^{-} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,co2}} \cdot S_{\mathrm{co2}}\right) \\ k_{\mathrm{A/Bin}} \cdot \left(S_{\mathrm{nh3}} \cdot c\left(\mathrm{H}^{+}\right) - K_{\mathrm{a,in}} \cdot S_{\mathrm{nh4}}^{+}\right) \\ k_{\mathrm{L}}a_{\mathrm{h2}} \cdot \left(S_{\mathrm{h2}} - \mathrm{pi}_{\mathrm{Sh2}} \cdot \frac{16}{R \cdot T \cdot K_{\mathrm{H,h2}}}\right) \cdot \frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}} \\ k_{\mathrm{L}}a_{\mathrm{ch4}} \cdot \left(S_{\mathrm{ch4}} - \mathrm{pi}_{\mathrm{Sch4}} \cdot \frac{64}{R \cdot T \cdot K_{\mathrm{H,ch4}}}\right) \cdot \frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}} \\ k_{\mathrm{L}}a_{\mathrm{co2}} \cdot \left(S_{\mathrm{co2}} - \mathrm{pi}_{\mathrm{Sco2}} \cdot \frac{1}{R \cdot T \cdot K_{\mathrm{H,co2}}}\right) \cdot \frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}} \\ k_{\mathrm{p}} \cdot \left(\mathrm{p}_{\mathrm{total}} - p_{\mathrm{ext}}\right) \cdot \frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}} \end{pmatrix} \tag{C.3}$$

$$
\begin{aligned}
f_{\mathrm{xi,Xc}} &:= 1 - f_{\mathrm{si,Xc}} - f_{\mathrm{ch,Xc}} - f_{\mathrm{pr,Xc}} - f_{\mathrm{li,Xc}} - f_{\mathrm{xp,Xc}} \\
f_{\mathrm{co2,Xc}} &:= C_{\mathrm{Xc}} - f_{\mathrm{si,Xc}} \cdot C_{\mathrm{SI}} - f_{\mathrm{ch,Xc}} \cdot C_{\mathrm{Xch}} - f_{\mathrm{pr,Xc}} \cdot C_{\mathrm{Xpr}} - f_{\mathrm{li,Xc}} \cdot C_{\mathrm{Xli}} - f_{\mathrm{xi,Xc}} \cdot C_{\mathrm{XI}} - f_{\mathrm{xp,Xc}} \cdot C_{\mathrm{Xp}} \\
f_{\mathrm{co2,Xli}} &:= C_{\mathrm{Xli}} - f_{\mathrm{fa,li}} \cdot C_{\mathrm{fa}} - \left(1 - f_{\mathrm{fa,li}}\right) \cdot C_{\mathrm{Xch}} \\
f_{\mathrm{ac,su}} &:= 1 - f_{\mathrm{h2,su}} - f_{\mathrm{bu,su}} - f_{\mathrm{pro,su}} \\
f_{\mathrm{co2,su}} &:= C_{\mathrm{Xch}} - \left(f_{\mathrm{bu,su}} \cdot C_{\mathrm{bu}} + f_{\mathrm{pro,su}} \cdot C_{\mathrm{pro}} + f_{\mathrm{ac,su}} \cdot C_{\mathrm{ac}}\right) \cdot (1 - Y_{\mathrm{su}}) - Y_{\mathrm{su}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{ac,aa}} &:= 1 - f_{\mathrm{h2,aa}} - f_{\mathrm{va,aa}} - f_{\mathrm{bu,aa}} - f_{\mathrm{pro,aa}} \\
f_{\mathrm{co2,aa}} &:= C_{\mathrm{Xpr}} - \left(f_{\mathrm{va,aa}} \cdot C_{\mathrm{va}} + f_{\mathrm{bu,aa}} \cdot C_{\mathrm{bu}} + f_{\mathrm{pro,aa}} \cdot C_{\mathrm{pro}} + f_{\mathrm{ac,aa}} \cdot C_{\mathrm{ac}}\right) \cdot (1 - Y_{\mathrm{aa}}) - Y_{\mathrm{aa}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{ac,fa}} &:= 1 - f_{\mathrm{h2,fa}} \\
f_{\mathrm{co2,fa}} &:= C_{\mathrm{fa}} - f_{\mathrm{ac,fa}} \cdot C_{\mathrm{ac}} \cdot (1 - Y_{\mathrm{fa}}) - Y_{\mathrm{fa}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{ac,va}} &:= 1 - f_{\mathrm{pro,va}} - f_{\mathrm{h2,va}} \\
f_{\mathrm{co2,va}} &:= C_{\mathrm{va}} - (f_{\mathrm{pro,va}} \cdot C_{\mathrm{pro}} + f_{\mathrm{ac,va}} \cdot C_{\mathrm{ac}}) \cdot (1 - Y_{\mathrm{c4}}) - Y_{\mathrm{c4}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{ac,bu}} &:= 1 - f_{\mathrm{h2,bu}} \\
f_{\mathrm{co2,bu}} &:= C_{\mathrm{bu}} - f_{\mathrm{ac,bu}} \cdot C_{\mathrm{ac}} \cdot (1 - Y_{\mathrm{c4}}) - Y_{\mathrm{c4}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{ac,pro}} &:= 1 - f_{\mathrm{h2,pro}} \\
f_{\mathrm{co2,pro}} &:= C_{\mathrm{pro}} - (1 - Y_{\mathrm{pro}}) \cdot f_{\mathrm{ac,pro}} \cdot C_{\mathrm{ac}} - Y_{\mathrm{pro}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{co2,ac}} &:= C_{\mathrm{ac}} - (1 - Y_{\mathrm{ac}}) \cdot C_{\mathrm{ch4}} - Y_{\mathrm{ac}} \cdot C_{\mathrm{xb}} \\
f_{\mathrm{co2,h2}} &:= -(1 - Y_{\mathrm{h2}}) \cdot C_{\mathrm{ch4}} - Y_{\mathrm{h2}} \cdot C_{\mathrm{xb}}
\end{aligned}
\tag{C.4}
$$

Inhibition functions:

$$
\begin{aligned}
I_1 &:= I_{\mathrm{in}} \cdot I_{\mathrm{pH,a}} & I_{\mathrm{in}} &:= \frac{S_{\mathrm{nh4}}^{+} + S_{\mathrm{nh3}}}{S_{\mathrm{nh4}}^{+} + S_{\mathrm{nh3}} + K_{\mathrm{S,IN}}} & I_{\mathrm{NH3}} &:= \frac{K_{\mathrm{I,NH3}}}{K_{\mathrm{I,NH3}} + S_{\mathrm{nh3}}} \\
I_{\mathrm{H2,fa}} &:= \frac{K_{\mathrm{I,H2,fa}}}{K_{\mathrm{I,H2,fa}} + S_{\mathrm{h2}}} & I_{\mathrm{H2,c4}} &:= \frac{K_{\mathrm{I,H2,c4}}}{K_{\mathrm{I,H2,c4}} + S_{\mathrm{h2}}} & I_{\mathrm{H2,pro}} &:= \frac{K_{\mathrm{I,H2,pro}}}{K_{\mathrm{I,H2,pro}} + S_{\mathrm{h2}}} \\
K_{\mathrm{I,H,a}} &:= 10^{-\frac{1}{2}\left(\mathrm{pH_{UL,a}} + \mathrm{pH_{LL,a}}\right)} & K_{\mathrm{I,H,h2}} &:= 10^{-\frac{1}{2}\left(\mathrm{pH_{UL,h2}} + \mathrm{pH_{LL,h2}}\right)} & K_{\mathrm{I,H,ac}} &:= 10^{-\frac{1}{2}\left(\mathrm{pH_{UL,ac}} + \mathrm{pH_{LL,ac}}\right)} \\
I_{\mathrm{pH,a}} &:= \frac{K_{\mathrm{I,H,a}}^{2}}{c\left(\mathrm{H^{+}}\right)^{2} + K_{\mathrm{I,H,a}}^{2}} & I_{\mathrm{pH,h2}} &:= \frac{K_{\mathrm{I,H,h2}}^{3}}{c\left(\mathrm{H^{+}}\right)^{3} + K_{\mathrm{I,H,h2}}^{3}} & I_{\mathrm{pH,ac}} &:= \frac{K_{\mathrm{I,H,ac}}^{3}}{c\left(\mathrm{H^{+}}\right)^{3} + K_{\mathrm{I,H,ac}}^{3}}
\end{aligned}
\tag{C.5}
$$

$$
\begin{aligned}
f_{\mathrm{ch,xb}} &:= \frac{f_{\mathrm{ch,Xc}}}{f_{\mathrm{ch,Xc}} + f_{\mathrm{pr,Xc}} + f_{\mathrm{li,Xc}}} \cdot (1 - f_{\mathrm{P}}) \\
f_{\mathrm{pr,xb}} &:= \frac{f_{\mathrm{pr,Xc}}}{f_{\mathrm{ch,Xc}} + f_{\mathrm{pr,Xc}} + f_{\mathrm{li,Xc}}} \cdot (1 - f_{\mathrm{P}}) \\
f_{\mathrm{li,xb}} &:= \frac{f_{\mathrm{li,Xc}}}{f_{\mathrm{ch,Xc}} + f_{\mathrm{pr,Xc}} + f_{\mathrm{li,Xc}}} \cdot (1 - f_{\mathrm{P}}) \\
f_{\mathrm{sin,xb}} &:= N_{\mathrm{xb}} - f_{\mathrm{P}} \cdot N_{\mathrm{Xp}} - f_{\mathrm{pr,xb}} \cdot N_{\mathrm{aa}} \\
f_{\mathrm{co2,xb}} &:= C_{\mathrm{xb}} - f_{\mathrm{P}} \cdot C_{\mathrm{Xp}} - f_{\mathrm{ch,xb}} \cdot C_{\mathrm{Xch}} - f_{\mathrm{pr,xb}} \cdot C_{\mathrm{Xpr}} - f_{\mathrm{li,xb}} \cdot C_{\mathrm{Xli}} \\
Q_{\mathrm{gas}} &:= k_{\mathrm{P}} \cdot \frac{\mathrm{P_{total}} - p_{\mathrm{ext}}}{R \cdot T \cdot 44.643} \cdot V_{\mathrm{liq}}
\end{aligned}
\tag{C.6}
$$

Table C.3: ADM1 parameter values as in Tschepetzki and Ogurek (2010).

Parameter	Value	Unit	Description
N_{I}	$0.06/14$	$\mathrm{mol}/\mathrm{g_{COD}}$	nitrogen content of inerts
N_{aa}	$0.098/14$	$\mathrm{mol}/\mathrm{g_{COD}}$	nitrogen content of amino acids and proteins
N_{xb}	$0.08/14$	$\mathrm{mol}/\mathrm{g_{COD}}$	nitrogen content of biomass
N_{Xp}	$0.06/14$	$\mathrm{mol}/\mathrm{g_{COD}}$	nitrogen content of X_{p}
C_{Xc}, C_{Xp}	0.03	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of composites (X_{p})
C_{SI}, C_{XI}	0.03	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of soluble (particulate) inerts
C_{Xch}	0.0313	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of carbohydrates
C_{Xpr}	0.03	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of proteins
C_{Xli}	0.022	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of lipids
C_{fa}	0.0217	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of LCFA
C_{va}	0.024	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of valerate
C_{bu}	0.025	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of butyrate
C_{pro}	0.0268	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of propionate
C_{ac}	0.0313	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of acetate
C_{ch4}	0.0156	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of methane
C_{xb}	0.0313	$\mathrm{mol}/\mathrm{g_{COD}}$	carbon content of biomass
Y_{su}	0.1	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	yield uptake of sugars
Y_{aa}	0.08	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	yield uptake of amino acids
Y_{fa}, Y_{c4}, Y_{h2}	0.06	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	yield uptake of LCFA (butyrate and valerate, hydrogen)
Y_{pro}	0.04	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	yield uptake of propionate
Y_{ac}	0.05	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	yield uptake of acetate
$f_{\mathrm{fa,li}}$	0.95	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	fatty acids from lipids
$f_{\mathrm{h2,su}}$	0.19	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from sugars
$f_{\mathrm{bu,su}}$	0.13	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	butyrate from sugars
$f_{\mathrm{pro,su}}$	0.27	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	propionate from sugars
$f_{\mathrm{h2,aa}}$	0.06	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from amino acids
$f_{\mathrm{va,aa}}$	0.23	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	valerate from amino acids
$f_{\mathrm{bu,aa}}$	0.26	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	butyrate from amino acids
$f_{\mathrm{pro,aa}}$	0.05	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	propionate from amino acids
$f_{\mathrm{h2,fa}}$	0.3	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from LCFA
$f_{\mathrm{h2,va}}$	0.15	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from valerate
$f_{\mathrm{pro,va}}$	0.54	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	propionate from valerate
$f_{\mathrm{h2,bu}}$	0.2	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from butyrate
$f_{\mathrm{h2,pro}}$	0.43	$\mathrm{g_{COD}}/\mathrm{g_{COD}}$	hydrogen from propionate
f_{p}	0.08	100 %	fraction of biomass leading to particulate products
$K_{\mathrm{S,IN}}$	$1 \cdot 10^{-4}$	mol/l	half saturation coefficient of inorganic nitrogen
$K_{\mathrm{S,su}}$	0.5	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of sugars
$K_{\mathrm{S,aa}}$	0.3	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of amino acids
$K_{\mathrm{S,fa}}$	0.4	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of LCFA
$K_{\mathrm{S,c4}}$	0.2	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of valerate and butyrate
$K_{\mathrm{S,pro}}$	0.1	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of propionate
$K_{\mathrm{S,ac}}$	0.15	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of acetate
$K_{\mathrm{S,h2}}$	$7 \cdot 10^{-6}$	$\mathrm{g_{COD}}/\mathrm{l}$	half saturation coefficient of hydrogen
$k_{\mathrm{m,su}}$	30	1/d	max. uptake rate of sugars
$k_{\mathrm{m,aa}}$	50	1/d	max. uptake rate of amino acids
$k_{\mathrm{m,fa}}$	6	1/d	max. uptake rate of LCFA
$K_{\mathrm{I,H2,fa}}$	$5 \cdot 10^{-6}$	$\mathrm{g_{COD}}/\mathrm{l}$	hydrogen inhibition constant for LCFA uptake
$K_{\mathrm{I,H2,c4}}$	$1 \cdot 10^{-5}$	$\mathrm{g_{COD}}/\mathrm{l}$	hydrogen inhibition constant for valerate and butyrate uptake
$K_{\mathrm{I,H2,pro}}$	$3.5 \cdot 10^{-6}$	$\mathrm{g_{COD}}/\mathrm{l}$	hydrogen inhibition constant for propionate uptake
$K_{\mathrm{I,NH3}}$	0.0018	mol/l	free ammonia inhibition constant for acetate uptake
$\mathrm{pH_{UL,a}}$, $\mathrm{pH_{LL,a}}$	5.5, 4	–	upper (lower) pH limit for ρ_5 to ρ_{10}
$\mathrm{pH_{UL,ac}}$, $\mathrm{pH_{LL,ac}}$	7, 6	–	upper (lower) pH limit for ρ_{11}
$\mathrm{pH_{UL,h2}}$, $\mathrm{pH_{LL,h2}}$	6, 5	–	upper (lower) pH limit for ρ_{12}
$k_{\mathrm{dec,su}}$, $k_{\mathrm{dec,aa}}$	0.02	1/d	decay rate of X_{su}, X_{aa}
$k_{\mathrm{dec,fa}}$, $k_{\mathrm{dec,c4}}$	0.02	1/d	decay rate of X_{fa}, X_{c4}
$k_{\mathrm{dec,pro}}$, $k_{\mathrm{dec,ac}}$	0.02	1/d	decay rate of X_{pro}, X_{ac}
$k_{\mathrm{dec,h2}}$	0.02	1/d	decay rate of X_{h2}
$K_{\mathrm{a,va}}$	$10^{-4.86}$	mol/l	acid-base equilibrium coefficient of valerate
$K_{\mathrm{a,bu}}$	$10^{-4.82}$	mol/l	acid-base equilibrium coefficient of butyrate
$K_{\mathrm{a,pro}}$	$10^{-4.88}$	mol/l	acid-base equilibrium coefficient of propionate
$K_{\mathrm{a,ac}}$	$10^{-4.76}$	mol/l	acid-base equilibrium coefficient of acetate
$K_{\mathrm{a,co2}}$	$4.94 \cdot 10^{-7}$	mol/l	acid-base equilibrium coefficient of carbon dioxide
$K_{\mathrm{a,in}}$	$1.11 \cdot 10^{-9}$	mol/l	acid-base equilibrium coefficient of ammonia
$k_{\mathrm{A/Bva}}$, $k_{\mathrm{A/Bbu}}$, $k_{\mathrm{A/Bpro}}$	$1 \cdot 10^{8}$	kmol/d	acid base kinetic parameter (valerate, butyrate, propionate)
$k_{\mathrm{A/Bac}}$, $k_{\mathrm{A/Bco2}}$, $k_{\mathrm{A/Bin}}$	$1 \cdot 10^{8}$	kmol/d	acid base kinetic parameter (acetate, carbon dioxide, ammonia)
$k_{\mathrm{L}}a_{\mathrm{h2}}$, $k_{\mathrm{L}}a_{\mathrm{ch4}}$, $k_{\mathrm{L}}a_{\mathrm{co2}}$	200	1/d	gas-liquid transfer coefficient of hydrogen (methane, carbon dioxide)
$K_{\mathrm{H,co2}}$	$1/\left(0.0271 \cdot R \cdot [T]\right)$	$\mathrm{mol}/\left(\mathrm{bar} \cdot \mathrm{m}^3\right)$	Henry constant of carbon dioxide, $[T] \stackrel{!}{=} \mathrm{K}$
$K_{\mathrm{H,ch4}}$	$1/\left(0.00116 \cdot R \cdot [T]\right)$	$\mathrm{mol}/\left(\mathrm{bar} \cdot \mathrm{m}^3\right)$	Henry constant of methane, $[T] \stackrel{!}{=} \mathrm{K}$
$K_{\mathrm{H,h2}}$	$1/\left(7.38 \cdot 10^{-4} \cdot R \cdot [T]\right)$	$\mathrm{mol}/\left(\mathrm{bar} \cdot \mathrm{m}^3\right)$	Henry constant of hydrogen, $[T] \stackrel{!}{=} \mathrm{K}$
K_{hyd}	2.5	$\%_{\mathrm{FM}}$	inhibition constant of hydrolysis
n_{hyd}	2.3	100 %	inhibition index of hydrolysis
R	$8.31399 \cdot 10^{-2}$	$\mathrm{m}^3 \cdot \mathrm{bar}/\left(\mathrm{kmol} \cdot \mathrm{K}\right)$	gas constant
p_{ext}	$1.04 - 0.0084147 \cdot \exp\left(0.054 \cdot \{T\}\right)$	bar	external pressure, $[T] \stackrel{!}{=} {}^{o}\mathrm{C}$
k_{p}	10000	$\mathrm{m}^3/\left(\mathrm{m}^3 \cdot \mathrm{d}\right)$	proportional control constant for gas balance

Appendix D

Symbols and Abbreviations

General Symbols

Symbol	Description	Ref.
$\mathbf{1}_n$	$n \in \mathbb{N}_0$ dimensional identity matrix	C
$\mathbf{0}_{n\times m}$	$n \times m$ dimensional zero matrix, $n, m \in \mathbb{N}_0$	C
$t \in \mathbb{R}_0^+$	continuous time, can be real and simulated	2
$\tau \in \mathbb{R}_0^+$	some time	2
d	differential	
$\delta_{\mathrm{D}}(x) = \begin{cases} \infty & \text{if } x = 0 \\ 0 & \text{if } x \neq 0 \end{cases}, \quad \int_{-\infty}^{\infty} \delta_{\mathrm{D}}(x)\mathrm{d}x = 1$	Dirac delta "function" (distribution)	2
$\delta_{\alpha\beta} = \begin{cases} 0 & \text{if } \alpha \neq \beta \\ 1 & \text{if } \alpha = \beta \end{cases}$	Kronecker delta	4.2
$E\langle x \rangle$	expectation value of the process x	2
$\mathbb{N}_0 := \{0, 1, 2, ...\}$	set of natural numbers	
$\mathbb{N} := \{1, 2, 3, ...\}$	set of natural numbers without zero	
$\mathbb{R}$	set of real numbers	
$\mathbb{R}^+ : t > 0$	set of positive real numbers	
$\mathbb{R}_0^+ : t \geq 0$	set of positive real numbers including 0	

System Definition (Biogas Plant)

Symbol	Description	Ref.
$n_\mathrm{x} \in \mathbb{N}_0$	number of states of the real-world system	2
$i_\mathrm{x} \in \{1, \ldots, n_\mathrm{x}\}$	iterator for the number of states of the real-world system	2
$\mathcal{X}_{i_\mathrm{x}} \subseteq \mathbb{R}$	vector space of the i_xth state of the real-world system	2
$x_{i_\mathrm{x}} : \mathbb{R}^+ \to \mathcal{X}_{i_\mathrm{x}}$	i_xth state of the real-world system	2
$\mathcal{X} := (\mathcal{X}_{i_\mathrm{x}})^{n_\mathrm{x}} := \mathcal{X}_1 \times \cdots \times \mathcal{X}_{n_\mathrm{x}}$	n_x dimensional state space of the real-world system	2
$\boldsymbol{x} := (x_1, \ldots, x_{i_\mathrm{x}}, \ldots, x_{n_\mathrm{x}})^T$	state vector of the real-world system	2
$n_\mathrm{u} \in \mathbb{N}_0$	number of inputs of the real-world system	2
$i_\mathrm{u} \in \{1, \ldots, n_\mathrm{u}\}$	iterator for the number of inputs of the real-world system	2
$\mathcal{U}_{i_\mathrm{u}} \subseteq \mathbb{R}$	vector space of the i_uth input of the real-world system	2
$u_{i_\mathrm{u}} : \mathbb{R}^+ \to \mathcal{U}_{i_\mathrm{u}}$	i_uth input of the real-world system	2
$\mathcal{U} := (\mathcal{U}_{i_\mathrm{u}})^{n_\mathrm{u}} := \mathcal{U}_1 \times \cdots \times \mathcal{U}_{n_\mathrm{u}}$	n_u dimensional input space of the real-world system	2
$\boldsymbol{u} := (u_1, \ldots, u_{i_\mathrm{u}}, \ldots, u_{n_\mathrm{u}})^T$	input vector of the real-world system	2
${}^o\boldsymbol{x} : \mathbb{R}^+ \to \mathcal{X}$	open loop predicted state of the real-world system	(2.1)
${}^o\boldsymbol{x} := ({}^ox_1, \ldots, {}^ox_{i_\mathrm{x}}, \ldots, {}^ox_{n_\mathrm{x}})^T$	open loop predicted state of the real-world system	(2.1)
$\boldsymbol{f} : \mathcal{X} \times \mathcal{U} \times \mathbb{R}^{n_\omega} \to \mathcal{TX}$	model of the real-world system	(2.1)
$\mathcal{TX} \subseteq \mathbb{R}^{n_\mathrm{x}}$	tangential state space of the real-world system	2
$\boldsymbol{\omega} : \mathbb{R}^+ \to \mathbb{R}^{n_\omega}$, $n_\omega \in \mathbb{N}_0$	n_ω dimensional process noise of the model $\boldsymbol{f}$	2
$\boldsymbol{\Psi}_{\boldsymbol{\omega}} \in \mathbb{R}^{n_\omega \times n_\omega}$	covariance matrix of process noise	2
$\boldsymbol{\omega}(t) \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Psi}_{\boldsymbol{\omega}})$, $E\left\langle \boldsymbol{\omega}(t) \cdot \boldsymbol{\omega}^T(\tau) \right\rangle = \boldsymbol{\Psi}_{\boldsymbol{\omega}} \cdot \delta_\mathrm{D}(t - \tau)$	normal distribution, zero-mean, white and uncorrelated process noise	2
$\sigma_{\omega_{i_\mathrm{u}}} \in \mathbb{R}^+$	standard deviation of the i_uth process noise ω_{i_u}	4.4.3
$n_\mathrm{y} \in \mathbb{N}_0$	number of outputs of the real-world system	4
$i_\mathrm{y} \in \{1, \ldots, n_\mathrm{y}\}$	iterator for the number of outputs of the real-world system	4
$\mathcal{Y}_{i_\mathrm{y}} \subseteq \mathbb{R}$	vector space of the i_yth output of the real-world system	4
$y_{i_\mathrm{y}} : \mathbb{R}^+ \to \mathcal{Y}_{i_\mathrm{y}}$	i_yth output of the real-world system	4
$\mathcal{Y} := \left(\mathcal{Y}_{i_\mathrm{y}}\right)^{n_\mathrm{y}} := \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_{n_\mathrm{y}}$	n_y dimensional output space of the real-world system	4
$\boldsymbol{y} := \left(y_1, \ldots, y_{i_\mathrm{y}}, \ldots, y_{n_\mathrm{y}}\right)^T$	output vector of the real-world system	4
$\sigma_{v_{i_\mathrm{y}}} \in \mathbb{R}^+$	standard deviation of the i_yth measurement noise v_{i_y}	4.4.3

Model Predictive Control

Symbol	Description	Ref.
$n_\mathrm{o} \in \mathbb{N}_0$	number of objectives	(2.2)
$i_\mathrm{o} \in \{1, \ldots, n_\mathrm{o}\}$	iterator for the number of objectives	(2.3)
$\widetilde{\boldsymbol{J}} : \mathcal{X} \times \mathcal{U} \to \mathbb{R}^{n_\mathrm{o}}$	n_o dimensional objective function for continuous input	(2.2)
$\widetilde{\boldsymbol{J}} := \left(\widetilde{J}_1, \ldots, \widetilde{J}_{n_\mathrm{o}}\right)^T$, $\widetilde{J}_{i_\mathrm{o}} : \mathcal{X} \times \mathcal{U} \to \mathbb{R}$	n_o dimensional objective function for continuous input	(2.3)
$\boldsymbol{u}^* : \mathbb{R}^+ \to \mathcal{U}$	optimal input function for the real-world system	(2.5)
$T_\mathrm{p} \in \mathbb{R}^+$	prediction horizon	2.1
$T_\mathrm{c} \in \mathbb{R}^+$	control horizon	2.1
$\delta \in \mathbb{R}^+$	control sampling time	2.1
$t_k := k \cdot \delta,\ k = 0, 1, 2, \ldots$	discrete time t_k, control sampling instant k	(2.6)
${}^o\boldsymbol{u} : [t_k, t_k + T_\mathrm{p}] \to \mathcal{U}$	open loop input applied to the model $\boldsymbol{f}$	(2.7)
${}^o\boldsymbol{u} := ({}^o u_1, \ldots, {}^o u_{i_\mathrm{u}}, \ldots, {}^o u_{n_\mathrm{u}})^T$	open loop input applied to the model $\boldsymbol{f}$	(2.7)
${}^o\boldsymbol{u}_k^* : [t_k, t_k + T_\mathrm{p}] \to \mathcal{U}$	optimal open loop input applied to the model $\boldsymbol{f}$	(2.7)
$s_\mathrm{c} := \frac{T_\mathrm{c}}{\delta} \in \mathbb{N}_0$	number of steps of the piecewise constant input over the control horizon T_c	2.1
$\boldsymbol{u}_{i_\mathrm{u}} := (u_{i_\mathrm{u},1}, \ldots, u_{i_\mathrm{u},s_\mathrm{c}})^T \in (\mathcal{U}_{i_\mathrm{u}})^{s_\mathrm{c}}$	vector of $i = 1, \ldots, s_\mathrm{c}$ amplitudes $u_{i_\mathrm{u},i} \in \mathcal{U}_{i_\mathrm{u}}$	(2.9)
$\mathcal{U}_\mathcal{F} := (\mathcal{U}_1)^{s_\mathrm{c}} \times \cdots \times (\mathcal{U}_{i_\mathrm{u}})^{s_\mathrm{c}} \times \cdots \times (\mathcal{U}_{n_\mathrm{u}})^{s_\mathrm{c}}$	input space for piecewise constant input, this is the feasible region	(2.10)
$\underline{\boldsymbol{u}} := \left(\boldsymbol{u}_1^T, \ldots, \boldsymbol{u}_{i_\mathrm{u}}^T, \ldots, \boldsymbol{u}_{n_\mathrm{u}}^T\right)^T \in \mathcal{U}_\mathcal{F}$	vector of optimization variables	(2.10)
$n_\mathrm{v} := s_\mathrm{c} \cdot n_\mathrm{u} \in \mathbb{N}_0$	number of optimization variables	2.1
$i_\mathrm{v} \in \{1, \ldots, n_\mathrm{v}\}$	iterator for the number of optimization variables	2.1
$\boldsymbol{f}_\mathcal{U} : \mathcal{U}_\mathcal{F} \to \mathcal{U}$, ${}^o\boldsymbol{u} : [t_k, t_k + T_\mathrm{p}] \to \boldsymbol{f}_\mathcal{U}(\underline{\boldsymbol{u}})$	transformation from vector of decision variables to piecewise constant input	(2.11)
$\boldsymbol{J} : \mathcal{X} \times \mathcal{U}_\mathcal{F} \to \mathbb{R}^{n_\mathrm{o}}$	multi-objective function for piecewise constant input	(2.13)
$\widetilde{\boldsymbol{J}}({}^o\boldsymbol{x}(\tau), {}^o\boldsymbol{u}(\tau)) = \widetilde{\boldsymbol{J}}({}^o\boldsymbol{x}(\tau), \boldsymbol{f}_\mathcal{U}(\underline{\boldsymbol{u}})) =: \boldsymbol{J}({}^o\boldsymbol{x}(\tau), \underline{\boldsymbol{u}}),\ \forall \tau \in [t_k, t_k + T_\mathrm{p}]$	multi-objective function for piecewise constant input	(2.13)
$\boldsymbol{J} := (J_1, \ldots, J_{n_\mathrm{o}})^T$, $J_{i_\mathrm{o}} : \mathcal{X} \times \mathcal{U}_\mathcal{F} \to \mathbb{R}$	multi-objective function for piecewise constant input	(2.13)
$\boldsymbol{J}_\boldsymbol{x}(\underline{\boldsymbol{u}}) := \boldsymbol{J}({}^o\boldsymbol{x}(\tau), \underline{\boldsymbol{u}})$	multi-objective function for piecewise constant input (omitting ${}^o\boldsymbol{x}$)	(2.16)
$\boldsymbol{J}_\boldsymbol{x} : \mathcal{U}_\mathcal{F} \to \mathbb{R}^{n_\mathrm{o}}$, $\boldsymbol{J}_\boldsymbol{x} := (J_{\boldsymbol{x},1}, \ldots, J_{\boldsymbol{x},n_\mathrm{o}})^T$, $J_{\boldsymbol{x},i_\mathrm{o}} : \mathcal{U}_\mathcal{F} \to \mathbb{R}$	multi-objective function for piecewise constant input (omitting ${}^o\boldsymbol{x}$)	(2.16)
$\varpi_{i_\mathrm{o}} \in (0, 1),\ \sum_{i_\mathrm{o}=1}^{n_\mathrm{o}} \varpi_{i_\mathrm{o}} = 1$	weighting factors in weighted sum of optimization criteria	(2.19)

Multi-Objective Optimization

Symbol	Description	Ref.
$\mathcal{P}^* : \{\underline{\boldsymbol{u}} \in \mathcal{U}_\mathcal{F} \,\vert \underline{\boldsymbol{u}} \text{ is Pareto optimal}\}$	Pareto optimal set	2.3
$\mathcal{PF}^* := \{\boldsymbol{J}_\mathfrak{x}(\underline{\boldsymbol{u}}) \in \mathbb{R}^{n_\mathrm{o}} \vert \underline{\boldsymbol{u}} \in \mathcal{P}^*\}$	Pareto front	2.4
$Vol : \mathbb{R}^{n_\mathrm{o}} \to \mathbb{R}$	Lebesgue measure for a n_o dimensional set	3.1
$\boldsymbol{r} \in \mathbb{R}^{n_\mathrm{o}}$	reference point used in definition of hypervolume indicator	3.1
$I_\mathrm{H} : \mathbb{R}^{n_\mathrm{o}} \to \mathbb{R}$	hypervolume indicator for a n_o dimensional set	3.1
$d_\mathrm{n}(\boldsymbol{\phi}, \mathcal{A}) := \mathrm{card}\{\boldsymbol{a}_\mathcal{A} \in \mathcal{A} \vert \boldsymbol{a}_\mathcal{A} \prec \boldsymbol{\phi}\}$	number of dominating points	(3.1)
$\Delta I_\mathrm{H}(\boldsymbol{a}_\mathcal{A}, \mathcal{A}) := I_\mathrm{H}(\mathcal{A}) - I_\mathrm{H}(\mathcal{A} \backslash \{\boldsymbol{a}_\mathcal{A}\})$, $\boldsymbol{a}_\mathcal{A} \in \mathcal{A}$, $\mathcal{A} \subset \mathbb{R}^{n_\mathrm{o}}$	contributing hypervolume	(3.2)
$\mathcal{D} \subset \mathbb{R}^{n_\mathrm{v}}$, $\boldsymbol{\phi} \in \mathcal{D}$	set of dominated individuals $\boldsymbol{\phi}$	3
$\mathcal{P} \subset \mathbb{R}^{n_\mathrm{v}}$	population of an evolutionary algorithm	3
$\mu \in \mathbb{N}_0$	number of parents in an evolutionary algorithm	3
$\lambda \in \mathbb{N}_0$	number of offspring in an evolutionary algorithm	3
$\kappa = 0, 1, 2, \ldots$	iterator of an evolutionary algorithm	3

State Estimation: Part I

Symbol	Description	Ref.
$\boldsymbol{h} : \mathcal{X} \times \mathbb{R}^{n_\upsilon} \to \mathcal{Y}$	measurement function	(4.1)
$\boldsymbol{\upsilon} : \mathbb{R}^+ \to \mathbb{R}^{n_\upsilon},\ n_\upsilon \in \mathbb{N}_0$	n_υ dimensional measurement noise of the model $\boldsymbol{h}$	(4.1)
$\boldsymbol{\Psi}_{\boldsymbol{\upsilon}} \in \mathbb{R}^{n_\upsilon \times n_\upsilon}$	covariance matrix of measurement noise	(4.1)
$\boldsymbol{\upsilon}(t) \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Psi}_{\boldsymbol{\upsilon}})$, $E\left\langle \boldsymbol{\upsilon}(t) \cdot \boldsymbol{\upsilon}^T(\tau) \right\rangle = \boldsymbol{\Psi}_{\boldsymbol{\upsilon}} \cdot \delta_{\mathrm{D}}(t-\tau)$	normal distribution, zero-mean, white and uncorrelated measurement noise	(4.1)
$\delta_{\mathrm{u}} \in \mathbb{R}^+$	sampling time for input values	(4.2)
$\delta_{\mathrm{y}} \in \mathbb{R}^+$	sampling time for output (measurement) values	(4.2)
$N_{\delta_{\mathrm{u}}} := \frac{\delta}{\delta_{\mathrm{u}}} \in \mathbb{N}_0$	ratio of sampling times $\delta/\delta_{\mathrm{u}}$	(4.2)
$N_{\delta_{\mathrm{y}}} := \frac{\delta}{\delta_{\mathrm{y}}} \in \mathbb{N}_0$	ratio of sampling times $\delta/\delta_{\mathrm{y}}$	(4.2)
$\boldsymbol{F}_{\mathrm{E}} : \mathcal{Y}^{N_{\delta_{\mathrm{y}}} \cdot t_k} \times \mathcal{U}^{N_{\delta_{\mathrm{u}}} \cdot t_k} \to \mathcal{X}$	state calculation function	4.1
$\mathcal{Y}^{N_{\delta_{\mathrm{y}}} \cdot t_k} := \{\boldsymbol{y}(0), \boldsymbol{y}(\delta_{\mathrm{y}}), \ldots, \boldsymbol{y}(\delta), \boldsymbol{y}(\delta+\delta_{\mathrm{y}}), \ldots, \boldsymbol{y}(t_k)\}$	set of measurements until t_k	(4.3)
$\mathcal{U}^{N_{\delta_{\mathrm{u}}} \cdot t_k} := \{\boldsymbol{u}(0), \boldsymbol{u}(\delta_{\mathrm{u}}), \ldots, \boldsymbol{u}(\delta), \boldsymbol{y}(\delta+\delta_{\mathrm{u}}), \ldots, \boldsymbol{u}(t_k)\}$	set of inputs until t_k	(4.4)
$\hat{\boldsymbol{x}}_{\boldsymbol{F}_{\mathrm{E}}}(t_k) := \boldsymbol{F}_{\mathrm{E}}(\boldsymbol{y}(0), \ldots, \boldsymbol{y}(t_k), \boldsymbol{u}(0), \ldots, \boldsymbol{u}(t_k))$	best state estimate using $\boldsymbol{F}_{\mathrm{E}}$	(4.5)
$\tilde{\boldsymbol{F}}_{\mathrm{E}} : \mathcal{Y}^{N_{\mathrm{y}}+1} \times \mathcal{U}^{N_{\mathrm{u}}+1} \to \mathcal{X}$	state estimation function, approximation of $\boldsymbol{F}_{\mathrm{E}}$	4.1
$\hat{\boldsymbol{x}} : \mathbb{R}^+ \to \mathcal{X}$	state vector estimate	4
$N_{\mathrm{u}} \in \mathbb{N}_0$	number of moving average filters for input	4.1
$N_{\mathrm{y}} \in \mathbb{N}_0$	number of moving average filters for measurement (output)	4.1
$w_{\mathrm{u}} \in \mathcal{W}_{\mathrm{u}} \subset \mathbb{N}_0$	window size of moving average filters for input	4.1
$w_{\mathrm{y}} \in \mathcal{W}_{\mathrm{y}} \subset \mathbb{N}_0$	window size of moving average filters for measurement	4.1
$\boldsymbol{\Lambda}_{\mathrm{u}} : \mathcal{U}^{w_{\mathrm{u}}} \to \mathcal{U}$	moving average filter for input	(4.6)
$\boldsymbol{\Lambda}_{\mathrm{y}} : \mathcal{Y}^{w_{\mathrm{y}}} \to \mathcal{Y}$	moving average filter for output	(4.8)
$i_{\boldsymbol{\Lambda}_{\mathrm{u}}} \in \{1, \ldots, N_{\mathrm{u}}\}$	iterator for the number of moving average filter for input	4.1
$i_{\boldsymbol{\Lambda}_{\mathrm{y}}} \in \{1, \ldots, N_{\mathrm{y}}\}$	iterator for the number of moving average filter for output	4.1
$w_{\mathrm{u},i_{\boldsymbol{\Lambda}_{\mathrm{u}}}} \in \mathcal{W}_{\mathrm{u}} \subset \mathbb{N}_0$	window size of $i_{\boldsymbol{\Lambda}_{\mathrm{u}}}$ th moving average input filter	4.1
$w_{\mathrm{y}},_{i_{\boldsymbol{\Lambda}_{\mathrm{y}}}} \in \mathcal{W}_{\mathrm{y}} \subset \mathbb{N}_0$	window size of $i_{\boldsymbol{\Lambda}_{\mathrm{y}}}$ th moving average measurement filter	4.1
$\overline{\boldsymbol{u}}_{i_{\boldsymbol{\Lambda}_{\mathrm{u}}}} : \mathbb{R}^+ \to \mathcal{U}$	moving average value of input	(4.7)
$\overline{\boldsymbol{y}}_{i_{\boldsymbol{\Lambda}_{\mathrm{y}}}} : \mathbb{R}^+ \to \mathcal{Y}$	moving average value of output	(4.9)
$D := n_{\mathrm{y}} \cdot (N_{\mathrm{y}}+1) + n_{\mathrm{u}} \cdot (N_{\mathrm{u}}+1)$	dimension of original feature space	(4.11)
$d \in \mathbb{N}_0$	dimension of projected feature space	4.1.1.1
$\boldsymbol{Y} \in \mathbb{R}^{N \times D},\ N := k \cdot N_{\delta_{\mathrm{y}}} + 1$	data of input and output values for state estimation	(4.11)
$\boldsymbol{Y}_{\mathrm{T}} \in \mathbb{R}^{N_{\mathrm{T}} \times D},\ N_{\mathrm{T}} < N$	training data of input and output values for state estimation	4.1.1
$\boldsymbol{Y}_{\mathrm{V}} \in \mathbb{R}^{N_{\mathrm{V}} \times D},\ N_{\mathrm{V}} := N - N_{\mathrm{T}}$	validation data of input and output values for state estimation	4.1.1
$\boldsymbol{X} := (\boldsymbol{x}_{i_{\mathrm{x}}}, \ldots, \boldsymbol{x}_{n_{\mathrm{x}}}) \in \mathbb{R}^{N \times n_{\mathrm{x}}}$	data of state vector values for state estimation	(4.12)
$\boldsymbol{x}_{i_{\mathrm{x}}} \in \mathbb{R}^N$	data of state vector $i_{\mathrm{x}} = 1, \ldots, n_{\mathrm{x}}$ for state estimation	(4.12)
$C \in \mathbb{N}_0$	number of classes in the classification problem	4.1.1
$\boldsymbol{\vartheta}_{i_{\mathrm{x}}} \in \{1, ..., C\}^N$	clustered data of state vector $\boldsymbol{X}_{i_{\mathrm{x}}},\ i_{\mathrm{x}} = 1, \ldots, n_{\mathrm{x}}$	4.1.1

State Estimation: Part II (the methods)

Symbol	Description	Ref.
$\boldsymbol{A}_{\mathrm{LDA}} \in \mathbb{R}^{d \times D}$	transformation matrix of linear discriminant analysis	4.1.1.1
$\boldsymbol{Z} := \left(\boldsymbol{z}_1, \ldots, \boldsymbol{z}_{N_{\mathrm{T}}}\right) \in \mathbb{R}^{d \times N_{\mathrm{T}}}$	matrix of projected features of discriminant analysis	4.1.1.1
$\boldsymbol{S}_{\mathrm{T}} \in \mathbb{R}^{D \times D}$	total scatter-matrix of linear discriminant analysis	(4.13)
$\boldsymbol{S}_{\mathrm{B}} \in \mathbb{R}^{D \times D}$	between-class scatter-matrix of linear discriminant analysis	(4.13)
$\mathcal{F}$	function space of nonlinear GerDA transformations, defined by a DNN	4.1.1.2
$\boldsymbol{f}_{\mathrm{GerDA}} : \mathbb{R}^D \to \mathbb{R}^d,\ \boldsymbol{f}_{\mathrm{GerDA}} \in \mathcal{F}$	some nonlinear GerDA transformation	4.1.1.2
$\boldsymbol{f}^*_{\mathrm{GerDA}} : \mathbb{R}^D \to \mathbb{R}^d,\ \boldsymbol{f}^*_{\mathrm{GerDA}} \in \mathcal{F}$	optimal nonlinear GerDA transformation	4.1.1.2
$\boldsymbol{W}, \boldsymbol{b}$	weights and biases of GerDA	4.1.1.2
$t_j := j \cdot \delta_{\mathrm{y}},\ j = 0, 1, 2, \ldots$	discrete time t_j, control sampling instant j	(4.14)
$\boldsymbol{X}_j := \boldsymbol{X}(t_j) \quad \text{and} \quad \boldsymbol{x}_j := \boldsymbol{x}(t_j)$	simplified notation for any matrix $\boldsymbol{X}(t_j) \in \mathbb{R}^{m \times n}$ and vector $\boldsymbol{x}(t_j) \in \mathbb{R}^n$, $n, m \in \mathbb{N}$	4.2
$\boldsymbol{X}_k := \boldsymbol{X}(t_k) \quad \text{and} \quad \boldsymbol{x}_k := \boldsymbol{x}(t_k)$	simplified notation for any matrix $\boldsymbol{X}(t_k) \in \mathbb{R}^{m \times n}$ and vector $\boldsymbol{x}(t_k) \in \mathbb{R}^n$, $n, m \in \mathbb{N}$	4.2
$\hat{\boldsymbol{x}}_j^- := \hat{\boldsymbol{x}}\left(t_j^-\right) \in \mathcal{X}$	a priori state estimate of Kalman filter at time t_j^-	4.2
$\hat{\boldsymbol{x}}_j^+ := \hat{\boldsymbol{x}}\left(t_j^+\right) \in \mathcal{X}$	a posteriori state estimate of Kalman filter at time t_j^+	4.2
$\boldsymbol{P}_j^- := E\left\langle \left(\boldsymbol{x}_j^- - \hat{\boldsymbol{x}}_j^-\right) \cdot \left(\boldsymbol{x}_j^- - \hat{\boldsymbol{x}}_j^-\right)^T \right\rangle$ $\boldsymbol{P}_j^- \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\mathrm{x}}}$	a priori estimation error covariance matrix of Kalman filter at time t_j^-	(4.18)
$\boldsymbol{P}_j^+ := E\left\langle \left(\boldsymbol{x}_j^+ - \hat{\boldsymbol{x}}_j^+\right) \cdot \left(\boldsymbol{x}_j^+ - \hat{\boldsymbol{x}}_j^+\right)^T \right\rangle$ $\boldsymbol{P}_j^+ \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\mathrm{x}}}$	a posteriori estimation error covariance matrix of Kalman filter at time t_j^+	(4.18)
$\boldsymbol{A}_j := \frac{\partial \boldsymbol{f}}{\partial^o \boldsymbol{x}}\left(\hat{\boldsymbol{x}}_{j-1}^+, \boldsymbol{u}(t_j), \boldsymbol{0}\right) \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\mathrm{x}}}$	system matrix of linearized model of $\boldsymbol{f}$	(4.19)
$\boldsymbol{C}_j := \frac{\partial \boldsymbol{h}}{\partial^o \boldsymbol{x}}\left(\hat{\boldsymbol{x}}_{j-1}^+, \boldsymbol{0}\right) \in \mathbb{R}^{n_{\mathrm{y}} \times n_{\mathrm{x}}}$	measurement matrix of linearized model of $\boldsymbol{h}$	(4.19)
$\boldsymbol{E}_j := \frac{\partial \boldsymbol{f}}{\partial \boldsymbol{\omega}}\left(\hat{\boldsymbol{x}}_{j-1}^+, \boldsymbol{u}(t_j), \boldsymbol{0}\right) \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\omega}}$	process noise matrix of linearized model of $\boldsymbol{f}$	(4.19)
$\boldsymbol{F}_j := \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{\upsilon}}\left(\hat{\boldsymbol{x}}_{j-1}^+, \boldsymbol{0}\right) \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\upsilon}}$	measurement noise matrix of linearized model of $\boldsymbol{h}$	(4.19)
$\boldsymbol{K}_j^* \in \mathbb{R}^{n_{\mathrm{x}} \times n_{\mathrm{y}}}$	optimal discrete Kalman matrix	(4.20)
$\boldsymbol{x}_{\circ} \in \mathcal{X}$	optimization variable (initial state) of MHE	4.3
$\boldsymbol{x}_{\circ}{}^* \in \mathcal{X}$	optimal value of optimization variable of MHE	4.3
$\delta_{\mathrm{MHE}} := w_{\mathrm{MHE}} \cdot \delta_{\mathrm{y}} \in \mathbb{R}^+$	length of the moving horizon	(4.21)
$w_{\mathrm{MHE}} \in \mathbb{N}$	unit-less length of the horizon, measured in units of δ_{y}	(4.21)
$\tilde{w}_{\mathrm{MHE}} := \frac{1}{N \delta_{\mathrm{y}}} \cdot w_{\mathrm{MHE}} \in \mathbb{N}$	unit-less length of the horizon, measured in units of δ	(4.22)
$\tilde{\boldsymbol{x}} : \mathbb{R}^+ \to \mathcal{X}$	initial state estimate in MHE	(4.23)
$\tilde{\boldsymbol{x}}_{\circ} := {}^o\boldsymbol{x}\left(t_{k+1} - \delta_{\mathrm{MHE}}\right) \in \mathcal{X}$	simple version of initial state estimate in MHE	4.3
$\kappa_{\mathrm{MHE}} \in \mathbb{R}^+$	weighting factor of MHE	(4.23)
$\boldsymbol{x}_{\mathrm{LB}}, \boldsymbol{x}_{\mathrm{UB}} \in \mathcal{X}$	lower, upper boundary for optimization variable in MHE	(4.23)
$\boldsymbol{x}_{i_{\mathrm{x}},[j_1,j_2]}$	vector of samples of state vector component i_{x}	(4.26)
$\boldsymbol{x}_{i_{\mathrm{x}},[k_1,k_2]}$	vector of samples of state vector component i_{x}	(4.27)
$e_{\hat{\boldsymbol{x}},i_{\mathrm{x}}} \in \mathbb{R}^+$	performance measure of i_{x}th estimated state vector component $\hat{x}_{i_{\mathrm{x}}}$	(4.28)
$e_{\hat{\boldsymbol{x}}} := \frac{1}{n_{\mathrm{x}}} \cdot \sum_{i_{\mathrm{x}}=1}^{n_{\mathrm{x}}} e_{\hat{\boldsymbol{x}},i_{\mathrm{x}}} \in \mathbb{R}^+$	total performance measure of experiments in Section 4.4	(4.29)

Anaerobic Digestion

Symbol	Description	Ref.
ash	ash in substrate	7.2
$\mathrm{COD}_{\mathrm{total}}$	total chemical oxygen demand of a substrate	7.2.1
$\mathrm{COD}_{\mathrm{SX}}$	disintegrated particulate chemical oxygen demand of substrate	(7.9)
$\mathrm{COD}_{\mathrm{X}}$	particulate chemical oxygen demand of a substrate	7.2.1
$\mathrm{COD}_{\mathrm{filtrate}}$	total chemical oxygen demand in the filtrate of a substrate	7.2.1
$d = \frac{\mathrm{NDF-VS_{IN}} \cdot (1 - D_{\mathrm{VS}})}{\mathrm{NDF-ADL}} \in [0, 1]$	degradable part of cellulose and hemicellulose	(7.11)
$D := \frac{Q_{\mathrm{IN}}}{V_{\mathrm{liq}}}$	dilution rate of digester	(5.6)
$\boldsymbol{D}_u : \mathbb{R}^+ \to \mathbb{R}^{37\times 34}$ $\boldsymbol{D}_x : \mathbb{R}^+ \to \mathbb{R}^{37\times 37}$	input and state transition matrix of ADM1	(7.1)
$f_{\mathrm{ch,Xc}}$, $f_{\mathrm{pr,Xc}}$	carbohydrates, proteins in non-disintegrated part of particulate COD	(7.11)
$f_{\mathrm{li,Xc}}$, $f_{\mathrm{xi,Xc}}$	lipids, inerts in non-disintegrated part of particulate COD	(7.11)
$I : \mathbb{R}^{37} \to [0, 1]$	inhibition function of ADM1	7.1
$j \in \{1, \ldots, 29\}$	process rate index of ADM1	7.1
$j_{\mathrm{S}} : \{2, 3, 4\} \to \{\mathrm{ch}, \mathrm{pr}, \mathrm{li}\}$	bijective function	(7.5)
$k_{\mathrm{hyd,ch}}, k_{\mathrm{hyd,pr}}, k_{\mathrm{hyd,li}}$	hydrolysis rates for carbohydrates, protein and lipids	(7.5)
K_{hyd}	inhibition constant of hydrolysis	(7.5)
mol	unit of the amount of substance, called mole	5.3.1
M	molar mass	5.3.1
n_{hyd}	inhibition index of hydrolysis	(7.5)
p_{IN}	cost of substrate	7.2
pH, $\mathrm{pH_{IN}}$	pH of sludge in digester, of substrate	7.2
$Q := \frac{\mathrm{d}V}{\mathrm{d}t}$	volumetric flow rate of a material	(5.5)
Q_{IN}	volumetric flow rate of a substrate	(5.5)
Q_{FST}	volumetric flow rate of sludge flowing into final storage tank	(5.5)
$Q_{\mathrm{gas}}, Q_{\mathrm{h_2}}, Q_{\mathrm{ch_4}}, Q_{\mathrm{co_2}}$	volumetric flow rates of biogas, hydrogen, methane and CO_2	(7.3)
$r_{\mathrm{h_2}}, r_{\mathrm{ch_4}}, r_{\mathrm{co_2}}$	relative content of hydrogen, methane and carbon dioxide in biogas	(7.4)
RF, RP and RL	raw fiber, raw proteins and raw lipids of substrate	7.2
T, T_{IN}	temperature in digester, of substrate	5.3.8
TA, $\mathrm{TA_{IN}}$	total alkalinity in digester, of substrate	7.2
$\mathrm{ThOD_{ch}}$, $\mathrm{ThOD_{pr}}$, $\mathrm{ThOD_{li}}$, $\mathrm{ThOD_{l}}$	theoretical oxygen demand of carbohydrates, proteins, lipids, lignin	7.2.1
$\overline{\mathrm{ThOD}}$	weighted mean of ThOD of substrate feed, see eq. (7.6)	(7.6)
TS, $\mathrm{TS_{IN}}$	total solids of sludge in digester, of substrate	5.3.10
${}^{o}\boldsymbol{u}_{\mathrm{AD}} : \mathbb{R}^+ \to \mathbb{R}^{34}$	input vector of ADM1	(7.2)
$\boldsymbol{V} : \mathbb{R}^{37} \to \mathbb{R}^{29\times 37}$	stoichiometric matrix of ADM1	(7.1)
VS, $\mathrm{VS_{IN}}$	volatile solids of sludge in digester, of substrate	5.3.11
V_{liq}, V_{gas}	digester volume of liquid phase, of gas phase	(5.6)
VFA/TA	ratio of volatile fatty acids (intermediate alkalinity) over TA	7.3.3.8
${}^{o}\boldsymbol{x}_{\mathrm{AD}} : \mathbb{R}^+ \to \mathbb{R}^{37}$	state vector of ADM1	(7.2)
$\boldsymbol{\rho} : \mathbb{R}^{37} \to \mathbb{R}^{29}$	process rates of ADM1	(7.1)
$\rho_{\mathrm{IN}}, \rho_{\mathrm{digester}}$	density of substrate feed, of sludge in digester (eq. (7.20))	(7.6)

Performance Indicators (Section 7.3, Part I)

Symbol	Description	Ref.
A_{ground}, A_{roof}, A_{wall}	surface area of ground, area and wall of cylindrical digester	(7.42)
$c_{\text{substrate}}$	specific heat capacity of a substrate	(7.39)
d_{dig}	diameter of digester	(7.40)
d_{mix}	diameter of agitator	(7.20)
d_{pipe}	diameter of a pipe	(7.31)
ΔE_j	thermal energy released due to microbial activity in reaction j	(7.43)
E_{plant}	total profit of produced electrical and thermal energy	(7.46)
g	gravitational acceleration	(7.30)
h_{dig}	wall height of digester	(7.40)
Δh_{geo}	geodetic head of a pump	(7.30)
h_{roof}	height of digester roof	(7.41)
$h_{v,h}$	higher heating value of produced biogas	(7.19)
h_{v,h,h_2}, h_{v,h,ch_4}, h_{v,h,co_2}	higher heating values of biogas components H_2, CH_4 and CO_2	(7.19)
k_{ground}, k_{roof}, k_{wall}	heat transfer coefficient of digester ground, roof and wall	(7.42)
k_{pipe}	pipe roughness	(7.34)
K_{c}	consistency coefficient to calculate effective viscosity η_{eff}	(7.23)
l_{pipe}	transport distance of a pump	(7.30)
n_{mix}	rotation speed of agitator	(7.20)
n_{flow}	flow index to calculate effective viscosity η_{eff}	(7.24)
N_{p}	Newton (or power) number	(7.20)
p_{char}	specific energy value for typical solid supply unit	(7.38)
p_{el}	costs for consumed electrical energy	(7.46)
p_{th}	costs for produced thermal energy by heating	(7.46)
Δp_{L}	pressure loss in a pipe	(7.31)
P_{el}, P_{th}	produced electrical, thermal power of a CHP	(7.17)
$P_{\text{el,consume}}$	total consumed electrical energy per day	(7.44)
P_{mix}	mechanical power of agitator	(7.20)
P_{MIX}	electrical energy consumption of agitator	(7.28)
P_{diss}	dissipated power of agitator	(7.29)
$P_{\text{mic\_heat}}$	thermal energy production due to microbial activity	(7.43)
P_{pump}	electrical energy consumption of liquid substrate and sludge transport	(7.30)
P_{solids}	electrical energy consumption of solids substrate transport	(7.38)
$P_{\text{substrate}}$	thermal power needed to heat substrates	(7.39)
ΔP_{th}	daily thermal energy balance of a biogas plant	(7.45)
r_{EEG}	remuneration of produced electrical energy	(7.46)
r_{th}	virtual or real revenue of produced thermal energy	(7.46)
Re	Reynolds number	(7.21)
Re_{pipe}	Reynolds number of a stream in a pipe	(7.33)
v_{pipe}	velocity of a medium in a pipe	(7.32)

Performance Indicators (Section 7.3, Part II)

Symbol	Description	Ref.
$F_{1\mathrm{D}} := \sum_{i_\mathrm{o}=1}^{n_\mathrm{o}} \varpi_{i_\mathrm{o}} \cdot F_{i_\mathrm{o}}$	one-dimensional stage cost	(7.71)
$\boldsymbol{F} := (F_1, F_2)^T$	stage cost in NMPC objective function	(7.62)
$J_{1\mathrm{D}} := \sum_{i_\mathrm{o}=1}^{n_\mathrm{o}} \varpi_{i_\mathrm{o}} \cdot J_{i_\mathrm{o}}$	fitness value	(7.70)
$\boldsymbol{T}_\mathrm{penalty} := (T_{\mathrm{penalty},1}, T_{\mathrm{penalty},2})^T$	terminal cost (terminal penalty term) in NMPC objective function	(7.62)
α_T	temperature correction for effective viscosity η_eff	(7.25)
$\dot{\gamma}$	shear rate	(7.36)
η_eff	effective viscosity of sludge in digester	(7.22)
$\eta_\mathrm{eff,pipe}$	effective viscosity of a medium in a pipe	(7.35)
$\eta_\mathrm{el}, \eta_\mathrm{th}$	electrical, thermal degree of efficiency of a CHP	(7.17)
η_heat	degree of efficiency of a heating	(7.45)
η_w	viscosity of water	(7.35)
$\kappa_{T,1}, \kappa_{T,2} \in \mathbb{R}^+$	weighting factor of terminal cost $T_{\mathrm{penalty},1}, T_{\mathrm{penalty},2}$	(7.64)
$\kappa_{i_\mathrm{c}} \in \mathbb{R}^+$	weight of constraint $i_\mathrm{c} = 1, \ldots, n_\mathrm{c}$ in stage cost component F_2	(7.66)
λ_pipe	pressure loss coefficient of a medium in a pipe	(7.34)
$\rho_\mathrm{Ty} : \mathbb{R} \to \mathbb{R}^+$	Tukey biweight function	(7.69)
τ_mix	runtime of the stirrer	(7.28)
τ_pipe	shear stress	(7.37)

Abbreviations (A - G)

Abbreviation	Description	Ref.
ABP	agricultural biogas plant	6
AD	anaerobic digestion	5
ADF	acid detergent fiber	7.2
ADL	acid detergent lignin	7.2
ADM1	anaerobic digestion model no. 1	7.1
ADM1d	distributed anaerobic digestion model no. 1	6
AF	anaerobic filter	5.4.2
AFB	anaerobic fixed bed	5.4.2
AM1	anaerobic digestion model introduced by Bernard et al. (2001a)	6
ANN	artificial neural networks	6
ARMAX	autoregressive moving average model with exogenous inputs	6
BA	bicarbonate alkalinity	6
BSM2	benchmark simulation model no. 2 (for wastewater treatment)	6
CCM	corn-cob-mix	7.4
CH_4	methane	5.1
CHP	combined heat and power plant	7
CMA-ES	covariance matrix adaptation evolution strategy	9.3.1
CO_2	carbon dioxide	5.1
COD	chemical oxygen demand	5.3.3
CSTR	continuous stirred-tank reactor	5.4.1
CV	curriculum vitae	1
DACE	design and analysis of computer experiments	3.2
dB	decibel	4.4
DIN	German institute for standardization (deutsches Institut für Normung)	7.2
DLL	dynamic link library	B
DNN	deep neural network	4.1.1
EA	evolutionary algorithm	3.1.1
EEG	Renewable Energy Sources Act	7.3.2
EGSB	expanded granular sludge bed	5.4.2
EKF	extended Kalman filter	6
EN	European standards (europäische Normen)	7.2
EPEX SPOT	European power spot market	1
EPSAC	extended prediction self-adaptive control	6
EU	European Union	1
FBR	fluidized bed reactor	5.4.2
FM	fresh mass: mass of untreated material	5.3.5
HRT	hydraulic retention time of digester	5.3.6
GerDA	generalized discriminant analysis	4.1.1
GC	gas chromatography	7.2
GPS	whole crop silage (Ganzpflanzensilage)	7.4
GUI	graphical user interface	B

Abbreviations (H - Z)

Abbreviation	Description	Ref.
H_2	hydrogen	5.1
HTML	hypertext markup language	B
I/O	input/output	B
ID	identifier	9.3
ISO	international organization for standardization	7.2
LCA	life cycle assessment	7.3.4
LCFA	long chain fatty acid	7.1.1
LDA	linear discriminant analysis	4.1.1
LHS	Latin hypercube sampling	9.3.1
LQT	linear quadratic tracking	6
MATLAB®	matrix laboratory	B
MCR	misclassification rate	8
MHE	moving horizon estimation	4.3
MONMPC	multi-objective nonlinear model predictive control	2
NDF	neutral detergent fiber	7.2
NfE	nitrogen free extract	7.2
NFC	non fiber carbohydrates	7.2
NMPC	nonlinear model predictive control	2
O_2	oxygen	5.3.3
ODE	ordinary differential equation	7
OFMSW	organic fraction of municipal solid waste	1
OLR	organic loading rate of digester	5.3.7
P	proportional controller	6
PC	personal computer	9.3
PCA	principal component analysis	6
pCO_2	partial pressure of CO_2	6
PDE	partial differential equation	6.3
PI	proportional-integral controller	6
PID	proportional-integral-derivative controller	6
PLC	programmable logic controller	9.2
PSO	particle swarm optimization	6
RTO	real-time optimization	2
RMSE	root-mean-square error	4.4
SCFA	short chain fatty acid	7.2.1
SDE+	Renewable Energy Production Incentive Scheme	1
SMS-EGO	$\mathcal{S}$-metric selection-based efficient global optimization	3.2
SMS-EMOA	$\mathcal{S}$ metric selection evolutionary multi-objective optimization algorithm	3.1.1
SRT	sludge retention time	5.3.6
ThOD	theoretical oxygen demand	5.3.9
TOC	total organic carbon	6
UASB	upflow anaerobic sludge blanket	5.4.2
UASB-AF	upflow anaerobic sludge blanket-anaerobic filter	5.4.2
UV/Vis	ultraviolet-visible	9.2
VFA	volatile fatty acids	7.3.3.8
VSM	variable structure model	6
WW	wastewater	6