Standard values

Model parameters

Systematic simplification of the Anaerobic Digestion Model No. 1 (ADM1) – Model development and stoichiometric analysis

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Symbols

C	Carbon content	[mol C g^{-1} COD]
COD	Chemical oxygen demand	
f	Yield coefficient	[g COD g^{-1} COD]
k	First-order reaction constant	[d^{-1}]
K_a	Dissociation constant (acid)	[mol L^{-1}]
k_{AB}	Kinetic dissociation rate (acid/base)	[L mol^{-1} d^{-1}]
K_H	Henry's law constant	[mol L^{-1} bar^{-1}]
K_I	Inhibition constant	[g L^{-1}] | [g COD L^{-1}] | [mol L^{-1}]
k_{La}	Volumetric mass transfer coefficient	[d^{-1}]
k_m	Maximum uptake rate (Monod)	[g COD g^{-1} COD d^{-1}]
k_p	Pipe friction coefficient	[L bar^{-1} d^{-1}]
K_S	Half-saturation constant (Monod)	[g L^{-1}] | [g COD L^{-1}] | [mol L^{-1}]
K_w	Ionic product (water)	[mol L^{-1}]
N	Nitrogen content	[mol N g^{-1} COD]
p	Pressure	[bar]
pK_a	Negative logarithmic dissociation constant	[-]
pH_{LL} | pH_{UL}	Lower and upper pH limit	[-]
R	Ideal gas constant	[bar L mol^{-1} K^{-1}]
Y	Biomass yield coefficient	[g g^{-1}] | [g COD g^{-1} COD]
—		
μ_m	Maximum growth rate (Monod)	[d^{-1}]

Indices

aa	Amino acids | acido- and acetogenesis
ac	Acetic acid
atm	Atmosphere
bac	Microorganisms
bu	Butyric acid
c4	Valeric and butyric acid
ch	Carbohydrates
ch4	Methane
co2	Carbon dioxide
dec	Decay
dis	Disintegration
fa	Long-chain fatty acids
h2	Hydrogen
hyd	Hydrolysis
I	Inerts
IN	Inorganic nitrogen
li	Lipids
pr	Proteins
pro	Propionic acid
sI	Soluble inerts
su	Sugars
va	Valeric acid
xc	Particulate composites
xI	Particulate inerts

Table 1.1a: Model parameters of the original COD-based ADM1 [3]

Carbon and nitrogen contents								
C_{xc}	0.02786	[mol C g^{-1} COD]	C_{su}	0.0313	[mol C g^{-1} COD]	C_{ch4}	0.0156	[mol C g^{-1} COD]
C_{ch}	0.0313	[mol C g^{-1} COD]	C_{aa}	0.03	[mol C g^{-1} COD]	N_{xc}	0.0027	[mol N g^{-1} COD]
C_{pr}	0.03	[mol C g^{-1} COD]	C_{fa}	0.0217	[mol C g^{-1} COD]	N_{I}	0.0043	[mol N g^{-1} COD]
C_{li}	0.022	[mol C g^{-1} COD]	C_{va}	0.024	[mol C g^{-1} COD]	N_{bac}	0.0057	[mol N g^{-1} COD]
C_{xI}	0.03	[mol C g^{-1} COD]	C_{bu}	0.025	[mol C g^{-1} COD]	N_{aa}	0.007	[mol N g^{-1} COD]
C_{sI}	0.03	[mol C g^{-1} COD]	C_{pro}	0.0268	[mol C g^{-1} COD]			
C_{bac}	0.0313	[mol C g^{-1} COD]	C_{ac}	0.0313	[mol C g^{-1} COD]			
Stoichiometric coefficients								
$f_{ch,xc}$	0.2	[g COD g^{-1} COD]	$f_{fa,li}$	0.95	[g COD g^{-1} COD]	$f_{bu,aa}$	0.26	[g COD g^{-1} COD]
$f_{pr,xc}$	0.2	[g COD g^{-1} COD]	$f_{bu,su}$	0.13	[g COD g^{-1} COD]	$f_{va,aa}$	0.23	[g COD g^{-1} COD]
$f_{li,xc}$	0.3	[g COD g^{-1} COD]	$f_{pro,su}$	0.27	[g COD g^{-1} COD]	$f_{pro,aa}$	0.05	[g COD g^{-1} COD]
$f_{xI,xc}$	0.2	[g COD g^{-1} COD]	$f_{ac,su}$	0.41	[g COD g^{-1} COD]	$f_{ac,aa}$	0.04	[g COD g^{-1} COD]
$f_{sI,xc}$	0.1	[g COD g^{-1} COD]	$f_{h2,su}$	0.19	[g COD g^{-1} COD]	$f_{h2,aa}$	0.06	[g COD g^{-1} COD]
Microbial biomass yields								
Y_{su}	0.1	[g COD g^{-1} COD]	Y_{c4}	0.06	[g COD g^{-1} COD]	Y_{h2}	0.06	[g COD g^{-1} COD]
Y_{aa}	0.08	[g COD g^{-1} COD]	Y_{pro}	0.04	[g COD g^{-1} COD]			
Y_{fa}	0.06	[g COD g^{-1} COD]	Y_{ac}	0.05	[g COD g^{-1} COD]			
Kinetic parameters								
$k_{m,su}$	30	[g COD g^{-1} COD d^{-1}]	$K_{S,su}$	0.5	[g COD L^{-1}]	k_{dis}	0.5	[d^{-1}]
$k_{m,aa}$	50	[g COD g^{-1} COD d^{-1}]	$K_{S,aa}$	0.3	[g COD L^{-1}]	k_{ch}	10	[d^{-1}]
$k_{m,fa}$	6	[g COD g^{-1} COD d^{-1}]	$K_{S,fa}$	0.4	[g COD L^{-1}]	k_{pr}	10	[d^{-1}]
$k_{m,c4}$	20	[g COD g^{-1} COD d^{-1}]	$K_{S,c4}$	0.2	[g COD L^{-1}]	k_{li}	10	[d^{-1}]
$k_{m,pro}$	13	[g COD g^{-1} COD d^{-1}]	$K_{S,pro}$	0.1	[g COD L^{-1}]	k_{dec}	0.02	[d^{-1}]
$k_{m,ac}$	8	[g COD g^{-1} COD d^{-1}]	$K_{S,ac}$	0.15	[g COD L^{-1}]			
$k_{m,h2}$	35	[g COD g^{-1} COD d^{-1}]	$K_{S,h2}$	$7{\cdot}10^{-6}$	[g COD L^{-1}]			
Inhibition constants								
$K_{S,IN}$	0.0001	[mol L^{-1}]	$pH_{LL,aa}$	4	[-]	$pH_{UL,aa}$	5.5	[-]
$K_{I,h2,fa}$	$5{\cdot}10^{-6}$	[g COD L^{-1}]	$pH_{LL,ac}$	6	[-]	$pH_{UL,ac}$	7	[-]
$K_{I,h2,c4}$	$1{\cdot}10^{-5}$	[g COD L^{-1}]	$pH_{LL,h2}$	5	[-]	$pH_{UL,h2}$	6	[-]
$K_{I,h2,pro}$	$3.5{\cdot}10^{-6}$	[g COD L^{-1}]						
$K_{I,nh3}$	0.0018	[mol L^{-1}]						
Dissociation constants and rates [a,b]								
$K_{a,va}$	$1{\cdot}10^{-4.86}$	[mol L^{-1}]	$k_{AB,va}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]	K_{w}	$1{\cdot}10^{-13.7}$	[mol L^{-1}]
$K_{a,bu}$	$1{\cdot}10^{-4.82}$	[mol L^{-1}]	$k_{AB,bu}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,pro}$	$1{\cdot}10^{-4.88}$	[mol L^{-1}]	$k_{AB,pro}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,ac}$	$1{\cdot}10^{-4.76}$	[mol L^{-1}]	$k_{AB,ac}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,co2}$	$1{\cdot}10^{-6.29}$	[mol L^{-1}]	$k_{AB,co2}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,IN}$	$1{\cdot}10^{-8.87}$	[mol L^{-1}]	$k_{AB,IN}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			

Table 1.1b: Model parameters of the original COD-based ADM1 [3]

Physicochemical parameters [c,d]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[mol L^{-1} bar^{-1}]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^4$	[L bar^{-1} d^{-1}]	$K_{H,co2}$	0.025	[mol L^{-1} bar^{-1}]	p_{atm}	1.0133	[bar]
R	0.08315	[bar L mol^{-1} K^{-1}]	$K_{H,h2}$	0.00072	[mol L^{-1} bar^{-1}]			

[a] Dissociation constants K_a in mol L^{-1} at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].

[b] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].

[c] Calculation of water vapour pressure p_{h2o} based on [1].

[d] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

Table 1.2: Model parameters of the mass-based ADM1 (variable stoichiometric yield coefficients)

Microbial biomass yields								
Y_{su}	0.08	[g g^{-1}]	Y_{va}	0.09	[g g^{-1}]	Y_{ac}	0.04	[g g^{-1}]
Y_{aa}	0.09	[g g^{-1}]	Y_{bu}	0.08	[g g^{-1}]	Y_{h2}	0.34	[g g^{-1}]
Y_{fa}	0.12	[g g^{-1}]	Y_{pro}	0.04	[g g^{-1}]			
Kinetic parameters [a]								
$\mu_{m,su}$	3	[d^{-1}]	$K_{S,su}$	0.47	[g L^{-1}]	k_{ch}	0.25	[d^{-1}]
$\mu_{m,aa}$	4	[d^{-1}]	$K_{S,aa}$	0.20	[g L^{-1}]	k_{pr}	0.2	[d^{-1}]
$\mu_{m,fa}$	0.36	[d^{-1}]	$K_{S,fa}$	0.14	[g L^{-1}]	k_{li}	0.1	[d^{-1}]
$\mu_{m,va}$	1.2	[d^{-1}]	$K_{S,va}$	0.10	[g L^{-1}]	k_{dec}	0.02	[d^{-1}]
$\mu_{m,bu}$	1.2	[d^{-1}]	$K_{S,bu}$	0.11	[g L^{-1}]			
$\mu_{m,pro}$	0.52	[d^{-1}]	$K_{S,pro}$	0.07	[g L^{-1}]			
$\mu_{m,ac}$	0.4	[d^{-1}]	$K_{S,ac}$	0.14	[g L^{-1}]			
$\mu_{m,h2}$	2.1	[d^{-1}]	$K_{S,h2}$	$8.8{\cdot}10^{-7}$	[g L^{-1}]			
Inhibition constants								
$K_{S,IN}$	0.0017	[g L^{-1}]	$pH_{LL,aa}$	4	[-]	$pH_{UL,aa}$	5.5	[-]
$K_{I,h2,fa}$	$6.3{\cdot}10^{-7}$	[g L^{-1}]	$pH_{LL,ac}$	6	[-]	$pH_{UL,ac}$	7	[-]
$K_{I,h2,c4}$	$1.3{\cdot}10^{-6}$	[g L^{-1}]	$pH_{LL,h2}$	5	[-]	$pH_{UL,h2}$	6	[-]
$K_{I,h2,pro}$	$4.4{\cdot}10^{-7}$	[g L^{-1}]						
$K_{I,nh3}$	0.0306	[g L^{-1}]						
Dissociation constants and rates [b,c]								
$K_{a,va}$	$1{\cdot}10^{-4.86}$	[mol L^{-1}]	$k_{AB,va}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]	K_w	$1{\cdot}10^{-13.7}$	[mol L^{-1}]
$K_{a,bu}$	$1{\cdot}10^{-4.82}$	[mol L^{-1}]	$k_{AB,bu}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,pro}$	$1{\cdot}10^{-4.88}$	[mol L^{-1}]	$k_{AB,pro}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,ac}$	$1{\cdot}10^{-4.76}$	[mol L^{-1}]	$k_{AB,ac}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,co2}$	$1{\cdot}10^{-6.29}$	[mol L^{-1}]	$k_{AB,co2}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,IN}$	$1{\cdot}10^{-8.87}$	[mol L^{-1}]	$k_{AB,IN}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
Physicochemical parameters [d,e]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[mol L^{-1} bar^{-1}]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^4$	[L bar^{-1} d^{-1}]	$K_{H,co2}$	0.025	[mol L^{-1} bar^{-1}]	p_{atm}	1.0133	[bar]
R	0.08315	[bar L mol^{-1} K^{-1}]	$K_{H,h2}$	0.00072	[mol L^{-1} bar^{-1}]			

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]

[b] Dissociation constants K_a in mol L^{-1} at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].

[c] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].

[d] Calculation of water vapour pressure p_{h2o} based on [1].

[e] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

Table 1.3: Model parameters of the mass-based ADM1 (fixed stoichiometric yield coefficients)

Kinetic parameters [a]								
$\mu_{m,su}$	3	[d^{-1}]	$K_{S,su}$	0.47	[g L^{-1}]	k_{ch}	0.25	[d^{-1}]
$\mu_{m,aa}$	4	[d^{-1}]	$K_{S,aa}$	0.20	[g L^{-1}]	k_{pr}	0.2	[d^{-1}]
$\mu_{m,fa}$	0.36	[d^{-1}]	$K_{S,fa}$	0.14	[g L^{-1}]	k_{li}	0.1	[d^{-1}]
$\mu_{m,va}$	1.2	[d^{-1}]	$K_{S,va}$	0.10	[g L^{-1}]	k_{dec}	0.02	[d^{-1}]
$\mu_{m,bu}$	1.2	[d^{-1}]	$K_{S,bu}$	0.11	[g L^{-1}]			
$\mu_{m,pro}$	0.52	[d^{-1}]	$K_{S,pro}$	0.07	[g L^{-1}]			
$\mu_{m,ac}$	0.4	[d^{-1}]	$K_{S,ac}$	0.14	[g L^{-1}]			
$\mu_{m,h2}$	2.1	[d^{-1}]	$K_{S,h2}$	$8.8 \cdot 10^{-7}$	[g L^{-1}]			
Inhibition constants								
$K_{S,IN}$	0.0017	[g L^{-1}]	$pH_{LL,aa}$	4	[-]	$pH_{UL,aa}$	5.5	[-]
$K_{I,h2,fa}$	$6.3 \cdot 10^{-7}$	[g L^{-1}]	$pH_{LL,ac}$	6	[-]	$pH_{UL,ac}$	7	[-]
$K_{I,h2,c4}$	$1.3 \cdot 10^{-6}$	[g L^{-1}]	$pH_{LL,h2}$	5	[-]	$pH_{UL,h2}$	6	[-]
$K_{I,h2,pro}$	$4.4 \cdot 10^{-7}$	[g L^{-1}]						
$K_{I,nh3}$	0.0306	[g L^{-1}]						
Dissociation constants and rates [b,c]								
$K_{a,va}$	$1 \cdot 10^{-4.86}$	[mol L^{-1}]	$k_{AB,va}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]	K_w	$1 \cdot 10^{-13.7}$	[mol L^{-1}]
$K_{a,bu}$	$1 \cdot 10^{-4.82}$	[mol L^{-1}]	$k_{AB,bu}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,pro}$	$1 \cdot 10^{-4.88}$	[mol L^{-1}]	$k_{AB,pro}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,ac}$	$1 \cdot 10^{-4.76}$	[mol L^{-1}]	$k_{AB,ac}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,co2}$	$1 \cdot 10^{-6.29}$	[mol L^{-1}]	$k_{AB,co2}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,IN}$	$1 \cdot 10^{-8.87}$	[mol L^{-1}]	$k_{AB,IN}$	$1 \cdot 10^{10}$	[L mol^{-1} d^{-1}]			
Physicochemical parameters [d,e]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[mol L^{-1} bar^{-1}]	p_{h2o}	0.0657	[bar]
k_p	$5 \cdot 10^4$	[L bar^{-1} d^{-1}]	$K_{H,co2}$	0.025	[mol L^{-1} bar^{-1}]	p_{atm}	1.0133	[bar]
R	0.08315	[bar L mol^{-1} K^{-1}]	$K_{H,h2}$	0.00072	[mol L^{-1} bar^{-1}]			

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]

[b] Dissociation constants K_a in mol L^{-1} at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].

[c] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].

[d] Calculation of water vapour pressure p_{h2o} based on [1].

[e] Correction of HENRY coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the VAN'T HOFF equation [4, 1].

Table 1.4a: Model parameters of the mass-based ADM1-R1

Kinetic parameters [a]								
$\mu_{m,su}$	3	[d^{-1}]	$K_{S,su}$	0.47	[g L^{-1}]	k_{ch}	0.25	[d^{-1}]
$\mu_{m,aa}$	4	[d^{-1}]	$K_{S,aa}$	0.20	[g L^{-1}]	k_{pr}	0.2	[d^{-1}]
$\mu_{m,fa}$	0.36	[d^{-1}]	$K_{S,fa}$	0.14	[g L^{-1}]	k_{li}	0.1	[d^{-1}]
$\mu_{m,va}$	1.2	[d^{-1}]	$K_{S,va}$	0.10	[g L^{-1}]	k_{dec}	0.02	[d^{-1}]
$\mu_{m,bu}$	1.2	[d^{-1}]	$K_{S,bu}$	0.11	[g L^{-1}]			
$\mu_{m,pro}$	0.52	[d^{-1}]	$K_{S,pro}$	0.07	[g L^{-1}]			
$\mu_{m,ac}$	0.4	[d^{-1}]	$K_{S,ac}$	0.14	[g L^{-1}]			
Inhibition constants								
$K_{S,IN}$	0.0017	[g L^{-1}]	$pH_{LL,aa}$	4	[-]	$pH_{UL,aa}$	5.5	[-]
$K_{I,nh3}$	0.0306	[g L^{-1}]	$pH_{LL,ac}$	6	[-]	$pH_{UL,ac}$	7	[-]

Table 1.4b: Model parameters of the mass-based ADM1-R1

Dissociation constants and rates [b,c]								
$K_{a,va}$	$1{\cdot}10^{-4.86}$	[mol L^{-1}]	$k_{AB,va}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]	K_w	$1{\cdot}10^{-13.7}$	[mol L^{-1}]
$K_{a,bu}$	$1{\cdot}10^{-4.82}$	[mol L^{-1}]	$k_{AB,bu}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,pro}$	$1{\cdot}10^{-4.88}$	[mol L^{-1}]	$k_{AB,pro}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,ac}$	$1{\cdot}10^{-4.76}$	[mol L^{-1}]	$k_{AB,ac}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,co2}$	$1{\cdot}10^{-6.29}$	[mol L^{-1}]	$k_{AB,co2}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,IN}$	$1{\cdot}10^{-8.87}$	[mol L^{-1}]	$k_{AB,IN}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
Physicochemical parameters [d,e]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[mol L^{-1} bar^{-1}]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^{4}$	[L bar^{-1} d^{-1}]	$K_{H,co2}$	0.025	[mol L^{-1} bar^{-1}]	p_{atm}	1.0133	[bar]
R	0.08315	[bar L mol^{-1} K^{-1}]						

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]
[b] Dissociation constants K_a in mol L^{-1} at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].
[c] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].
[d] Calculation of water vapour pressure p_{h2o} based on [1].
[e] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

Table 1.5: Model parameters of the mass-based ADM1-R2

Kinetic parameters [a]								
$\mu_{m,va}$	1.2	[d^{-1}]	$K_{S,va}$	0.10	[g L^{-1}]	k_{ch}	0.25	[d^{-1}]
$\mu_{m,bu}$	1.2	[d^{-1}]	$K_{S,bu}$	0.11	[g L^{-1}]	k_{pr}	0.2	[d^{-1}]
$\mu_{m,pro}$	0.52	[d^{-1}]	$K_{S,pro}$	0.07	[g L^{-1}]	k_{li}	0.1	[d^{-1}]
$\mu_{m,ac}$	0.4	[d^{-1}]	$K_{S,ac}$	0.14	[g L^{-1}]	k_{dec}	0.02	[d^{-1}]
Inhibition constants								
$K_{S,IN}$	0.0017	[g L^{-1}]	$pH_{LL,aa}$	4	[-]	$pH_{UL,aa}$	5.5	[-]
$K_{I,nh3}$	0.0306	[g L^{-1}]	$pH_{LL,ac}$	6	[-]	$pH_{UL,ac}$	7	[-]
Dissociation constants and rates [b,c]								
$K_{a,va}$	$1{\cdot}10^{-4.86}$	[mol L^{-1}]	$k_{AB,va}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]	K_w	$1{\cdot}10^{-13.7}$	[mol L^{-1}]
$K_{a,bu}$	$1{\cdot}10^{-4.82}$	[mol L^{-1}]	$k_{AB,bu}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,pro}$	$1{\cdot}10^{-4.88}$	[mol L^{-1}]	$k_{AB,pro}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,ac}$	$1{\cdot}10^{-4.76}$	[mol L^{-1}]	$k_{AB,ac}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,co2}$	$1{\cdot}10^{-6.29}$	[mol L^{-1}]	$k_{AB,co2}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
$K_{a,IN}$	$1{\cdot}10^{-8.87}$	[mol L^{-1}]	$k_{AB,IN}$	$1{\cdot}10^{10}$	[L mol^{-1} d^{-1}]			
Physicochemical parameters [d,e]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[mol L^{-1} bar^{-1}]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^{4}$	[L bar^{-1} d^{-1}]	$K_{H,co2}$	0.025	[mol L^{-1} bar^{-1}]	p_{atm}	1.0133	[bar]
R	0.08315	[bar L mol^{-1} K^{-1}]						

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]
[b] Dissociation constants K_a in mol L^{-1} at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].
[c] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].
[d] Calculation of water vapour pressure p_{h2o} based on [1].
[e] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

Table 1.6: Model parameters of the mass-based ADM1-R3

Kinetic parameters [a]								
$\mu_{m,ac}$	0.4	[d^{-1}]	k_{ch}	0.25	[d^{-1}]	k_{li}	0.1	[d^{-1}]
$K_{S,ac}$	0.14	[$g\,L^{-1}$]	k_{pr}	0.2	[d^{-1}]	k_{dec}	0.02	[d^{-1}]
Inhibition constants								
$K_{S,IN}$	0.0017	[$g\,L^{-1}$]	$pH_{LL,ac}$	6	[-]			
$K_{I,nh3}$	0.0306	[$g\,L^{-1}$]	$pH_{UL,ac}$	7	[-]			
Dissociation constants and rates [b,c]								
$K_{a,ac}$	$1{\cdot}10^{-4.76}$	[$mol\,L^{-1}$]	$k_{AB,ac}$	$1{\cdot}10^{10}$	[$L\,mol^{-1}\,d^{-1}$]	K_w	$1{\cdot}10^{-13.7}$	[$mol\,L^{-1}$]
$K_{a,co2}$	$1{\cdot}10^{-6.29}$	[$mol\,L^{-1}$]	$k_{AB,co2}$	$1{\cdot}10^{10}$	[$L\,mol^{-1}\,d^{-1}$]			
$K_{a,IN}$	$1{\cdot}10^{-8.87}$	[$mol\,L^{-1}$]	$k_{AB,IN}$	$1{\cdot}10^{10}$	[$L\,mol^{-1}\,d^{-1}$]			
Physicochemical parameters [d,e]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[$mol\,L^{-1}\,bar^{-1}$]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^4$	[$L\,bar^{-1}\,d^{-1}$]	$K_{H,co2}$	0.025	[$mol\,L^{-1}\,bar^{-1}$]	p_{atm}	1.0133	[bar]
R	0.08315	[$bar\,L\,mol^{-1}\,K^{-1}$]						

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]

[b] Dissociation constants K_a in $mol\,L^{-1}$ at 293.15 K (20°C) and $K_a = 1 \cdot 10^{-pK_a}$ according to [2].

[c] Correction for mesophilic process temperatures at 311.15 K (38°C) according to [3].

[d] Calculation of water vapour pressure p_{h2o} based on [1].

[e] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

Table 1.7: Model parameters of the mass-based ADM1-R4

Kinetic parameters [a]								
k_{ch}	0.25	[d^{-1}]	k_{li}	0.1	[d^{-1}]			
k_{pr}	0.2	[d^{-1}]	k_{dec}	0.02	[d^{-1}]			
Physicochemical parameters [b,c]								
k_{La}	200	[d^{-1}]	$K_{H,ch4}$	0.0011	[$mol\,L^{-1}\,bar^{-1}$]	p_{h2o}	0.0657	[bar]
k_p	$5{\cdot}10^4$	[$L\,bar^{-1}\,d^{-1}$]	$K_{H,co2}$	0.025	[$mol\,L^{-1}\,bar^{-1}$]	p_{atm}	1.0133	[bar]
R	0.08315	[$bar\,L\,mol^{-1}\,K^{-1}$]						

[a] Recommended first-order reaction constants for mesophilic (high-rate) hydrolysis of individual nutrients [1]

[b] Calculation of water vapour pressure p_{h2o} based on [1].

[s] Correction of Henry coefficients $K_{H,i}$ for mesophilic process temperatures at 311.15 K (38°C) based on the van't Hoff equation [4, 1].

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