Petersen matrices

Modell structures

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

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Symbols

a | b | c	Universal constants and parameters	
C	Carbon content	[mol C g^{-1} COD]
COD	Chemical oxygen demand	
D	Dilution rate	[d^{-1}]
f	Yield coefficient	[g g^{-1}] | [g COD g^{-1} COD]
HRT	Hydraulic retention time	[d]
I	Inhibition function	[-]
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	[-]
q	Volume flow at standard conditions (293 K and 1.01325 bar)	[L d^{-1}]
R	Ideal gas constant	[bar L mol^{-1} K^{-1}]
S	Soluble or gaseous component (state variable)	[g L^{-1}] | [g COD L^{-1}] | [mol L^{-1}]
T	Temperature	[K]
V	Volume	[L]
v	Stoichiometric biogas or methane potential	[L kg^{-1}]
X	Particulate component (state variable)	[g L^{-1}] | [g COD L^{-1}] | [mol L^{-1}]
Y	Biomass yield coefficient	[g g^{-1}] | [g COD g^{-1} COD]
—		
μ_m	Maximum growth rate (Monod)	[d^{-1}]
ν	Stoichiometric coefficient	[-] | [g COD L^{-1}]
ρ	Process rate | Reaction rate	[g L^{-1} d^{-1}] | [g COD L^{-1} d^{-1}] | [mol L^{-1} d^{-1}]
ρ_T	Transfer rate (phase transition)	[g L^{-1} d^{-1}] | [g COD L^{-1} d^{-1}] | [mol L^{-1} d^{-1}]

Indices

aa	Amino acids | acido- and acetogenesis
ac	Acetic acid
an^-	Anions
atm	Atmosphere
bac	Microorganisms
bu	Butyric acid
c4	Valeric and butyric acid
cat^+	Cations
ch	Carbohydrates
ch4	Methane
co2	Carbon dioxide
dec	Decay
dis	Disintegration
fa	Long-chain fatty acids
gas	Gas phase
h2	Hydrogen
hyd	Hydrolysis
I	Inerts
IC	Inorganic carbon
IN	Inorganic nitrogen
li	Lipids
liq	Liquid phase | solid-liquid phase
pr	Proteins
pro	Propionic acid
sI	Soluble inerts
su	Sugars
va	Valeric acid
X	Microorganisms
xc	Particulate composites
xI	Particulate inerts

Table 1.1a: Model structure of the original COD-based ADM1 [1]

Component i →	1	2	3	4	5	6	7	8	9	10	11	
j Process ↓	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	S_{IC}	S_{IN}	**Process rate** ρ_j
1 Disintegration X_c										$-\sum C_i \nu_{i,1}$	N_{xc}-$f_{pr,xc}$ N_{aa}	$k_{dis} X_c$
2 Hydrolysis X_{ch}	1									C_{ch}-C_{su}		$k_{ch} X_{ch}$
3 Hydrolysis X_{pr}		1								C_{pr}-C_{aa}		$k_{pr} X_{pr}$
4 Hydrolysis X_{li}	1-$f_{fa,li}$		$f_{fa,li}$							$-\sum C_i \nu_{i,4}$		$k_{li} X_{li}$
5 Acidogenesis S_{su}	-1				$(1\text{-}Y_{su})\, f_{bu,su}$	$(1\text{-}Y_{su})\, f_{pro,su}$	$(1\text{-}Y_{su})\, f_{ac,su}$	$(1\text{-}Y_{su})\, f_{h2,su}$		$-\sum C_i \nu_{i,5}$	-Y_{su} N_{bac}	$k_{m,su} \frac{S_{su}}{K_{S,su}+S_{su}} X_{su} I_{su}$
6 Acidogenesis S_{aa}		-1		$(1\text{-}Y_{aa})\, f_{va,aa}$	$(1\text{-}Y_{aa})\, f_{bu,aa}$	$(1\text{-}Y_{aa})\, f_{pro,aa}$	$(1\text{-}Y_{aa})\, f_{ac,aa}$	$(1\text{-}Y_{aa})\, f_{h2,aa}$		$-\sum C_i \nu_{i,6}$	N_{aa}-Y_{aa} N_{bac}	$k_{m,aa} \frac{S_{aa}}{K_{S,aa}+S_{aa}} X_{aa} I_{aa}$
7 Acidogenesis S_{fa}			-1				$(1\text{-}Y_{fa})\, 0,7$	$(1\text{-}Y_{fa})\, 0,3$		$-\sum C_i \nu_{i,7}$	-Y_{fa} N_{bac}	$k_{m,fa} \frac{S_{fa}}{K_{S,fa}+S_{fa}} X_{fa} I_{fa}$
8 Acetogenesis S_{va}				-1		$(1\text{-}Y_{c4})\, 0,54$	$(1\text{-}Y_{c4})\, 0,31$	$(1\text{-}Y_{c4})\, 0,15$		$-\sum C_i \nu_{i,8}$	-Y_{c4} N_{bac}	$k_{m,c4} \frac{S_{va}}{K_{S,c4}+S_{va}} \frac{X_{c4}\, S_{va}}{S_{va}+S_{bu}} I_{c4}$
9 Acetogenesis S_{bu}					-1		$(1\text{-}Y_{c4})\, 0,8$	$(1\text{-}Y_{c4})\, 0,2$		$-\sum C_i \nu_{i,9}$	-Y_{c4} N_{bac}	$k_{m,c4} \frac{S_{bu}}{K_{S,c4}+S_{bu}} \frac{X_{c4}\, S_{bu}}{S_{bu}+S_{va}} I_{c4}$
10 Acetogenesis S_{pro}						-1	$(1\text{-}Y_{pro})\, 0,57$	$(1\text{-}Y_{pro})\, 0,43$		$-\sum C_i \nu_{i,10}$	-Y_{pro} N_{bac}	$k_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro} I_{pro}$
11 Methanogenesis S_{ac}							-1		1-Y_{ac}	$-\sum C_i \nu_{i,11}$	-Y_{ac} N_{bac}	$k_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac} I_{ac}$
12 Methanogenesis S_{h2}								-1	1-Y_{h2}	$-\sum C_i \nu_{i,12}$	-Y_{h2} N_{bac}	$k_{m,h2} \frac{S_{h2}}{K_{S,h2}+S_{h2}} X_{h2} I_{h2}$
13 Decay X_{su}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{su}$
14 Decay X_{aa}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{aa}$
15 Decay X_{fa}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{fa}$
16 Decay X_{c4}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{c4}$
17 Decay X_{pro}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{pro}$
18 Decay X_{ac}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{ac}$
19 Decay X_{h2}										C_{bac}-C_{xc}	N_{bac}-N_{xc}	$k_{dec} X_{h2}$

Table 1.1b: Model structure of the original COD-based ADM1 [1]

Component i →	12	13	14	15	16	17	18	19	20	21	22	23	24	
j Process↓	S_I	X_c	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{c4}	X_{pro}	X_{ac}	X_{h2}	X_I	**Process rate** ρ_j
1 Disintegration	$f_{sI,xc}$	-1	$f_{ch,xc}$	$f_{pr,xc}$	$f_{li,xc}$								$f_{xI,xc}$	$k_{dis} \cdot X_c$
2 Hydrolysis X_{ch}			-1											$k_{ch}\, X_{ch}$
3 Hydrolysis X_{pr}				-1										$k_{pr}\, X_{pr}$
4 Hydrolysis X_{li}					-1									$k_{li}\, X_{li}$
5 Acidogenesis S_{su}						Y_{su}								$k_{m,su} \frac{S_{su}}{K_{S,su}+S_{su}} X_{su}\, I_{su}$
6 Acidogenesis S_{aa}							Y_{aa}							$k_{m,aa} \frac{S_{aa}}{K_{S,aa}+S_{aa}} X_{aa}\, I_{aa}$
7 Acidogenesis S_{fa}								Y_{fa}						$k_{m,fa} \frac{S_{fa}}{K_{S,fa}+S_{fa}} X_{fa}\, I_{fa}$
8 Acetogenesis S_{va}									Y_{c4}					$k_{m,c4} \frac{S_{va}}{K_{S,c4}+S_{va}} \frac{X_{c4}\, S_{va}}{S_{va}+S_{bu}} I_{c4}$
9 Acetogenesis S_{bu}									Y_{c4}					$k_{m,c4} \frac{S_{bu}}{K_{S,c4}+S_{bu}} \frac{X_{c4}\, S_{bu}}{S_{bu}+S_{va}} I_{c4}$
10 Acetogenesis S_{pro}										Y_{pro}				$k_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
11 Methanogenesis S_{ac}											Y_{ac}			$k_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
12 Methanogenesis S_{h2}												Y_{h2}		$k_{m,h2} \frac{S_{h2}}{K_{S,h2}+S_{h2}} X_{h2}\, I_{h2}$
13 Decay X_{su}		1				-1								$k_{dec}\, X_{su}$
14 Decay X_{aa}		1					-1							$k_{dec}\, X_{aa}$
15 Decay X_{fa}		1						-1						$k_{dec}\, X_{fa}$
16 Decay X_{c4}		1							-1					$k_{dec}\, X_{c4}$
17 Decay X_{pro}		1								-1				$k_{dec}\, X_{pro}$
18 Decay X_{ac}		1									-1			$k_{dec}\, X_{ac}$
19 Decay X_{h2}		1										-1		$k_{dec}\, X_{h2}$

Table 1.1c: Model structure of the original COD-based ADM1 [1]

Component i → / **j Process↓**	8 S_{h2}	9 S_{ch4}	10 S_{IC}	...	25 S_{an^-}	26 S_{cat^+}	27 S_{va^-}	28 S_{bu^-}	29 S_{pro^-}	30 S_{ac^-}	31 S_{hco3^-}	32 S_{nh3}	33 $S_{gas,h2}$	34 $S_{gas,ch4}$	35 $S_{gas,co2}$	**Process rate** ρ_j
20 Dissociation S_{va}							-1									$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+})-K_{a,va}\,S_{va})$
21 Dissociation S_{bu}								-1								$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+})-K_{a,bu}\,S_{bu})$
22 Dissociation S_{pro}									-1							$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+})-K_{a,pro}\,S_{pro})$
23 Dissociation S_{ac}										-1						$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+})-K_{a,ac}\,S_{ac})$
24 Dissociation S_{IC}											-1					$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+})-K_{a,co2}\,S_{IC})$
25 Dissociation S_{IN}												-1				$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+})-K_{a,IN}\,S_{IN})$
26 Phase transition S_{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{La}\,(S_{h2}-16\,K_{H,h2}\,p_{h2})$
27 Phase transition S_{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4}-64\,K_{H,ch4}\,p_{ch4})$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2}-K_{H,co2}\,p_{co2})$

Inhibition

$I_{su} = I_{aa} = I_{pH,aa}\,I_{IN,lim}$ $\quad I_{fa} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,fa}$ $\quad I_{c4} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,c4}$

$I_{pro} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,pro}$ $\quad I_{ac} = I_{pH,ac}\,I_{IN,lim}\,I_{nh3}$ $\quad I_{h2} = I_{pH,h2}\,I_{IN,lim}$

$I_{IN,lim} = \frac{S_{IN}}{S_{IN}+K_{S,IN}}$ $\quad I_{h2,fa} = \frac{K_{I,h2,fa}}{K_{I,h2,fa}+S_{h2}}$ $\quad I_{h2,c4} = \frac{K_{I,h2,c4}}{K_{I,h2,c4}+S_{h2}}$

$I_{h2,pro} = \frac{K_{I,h2,pro}}{K_{I,h2,pro}+S_{h2}}$ $\quad I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3}+S_{nh3}}$

$I_{pH,aa} = \frac{K_{pH,aa}^{n_{aa}}}{K_{pH,aa}^{n_{aa}}+S_{H^+}^{n_{aa}}}$ $\quad n_{aa} = \frac{3}{pH_{UL,aa}-pH_{LL,aa}}$ $\quad K_{pH,aa} = 10^{-\frac{pH_{UL,aa}+pH_{LL,aa}}{2}}$

$I_{pH,ac} = \frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}}+S_{H^+}^{n_{ac}}}$ $\quad n_{ac} = \frac{3}{pH_{UL,ac}-pH_{LL,ac}}$ $\quad K_{pH,ac} = 10^{-\frac{pH_{UL,ac}+pH_{LL,ac}}{2}}$

$I_{pH,h2} = \frac{K_{pH,h2}^{n_{h2}}}{K_{pH,aa}^{n_{h2}}+S_{H^+}^{n_{h2}}}$ $\quad n_{h2} = \frac{3}{pH_{UL,h2}-pH_{LL,h2}}$ $\quad K_{pH,h2} = 10^{-\frac{pH_{UL,h2}+pH_{LL,h2}}{2}}$

Algebraic equations

$S_{nh4^+} = S_{IN} - S_{nh3}$ $\quad S_{co2} = S_{IC} - S_{hco3^-}$

$\phi = S_{cat^+} + S_{nh4^+} - S_{hco3^-} - \frac{S_{ac^-}}{64} + \frac{S_{pro^-}}{112} - \frac{S_{bu^-}}{160} - \frac{S_{va^-}}{208} - S_{an^-}$

$S_{H^+} = -\frac{\phi}{2} + \frac{1}{2}\sqrt{\phi^2+4\,K_w}$ $\quad pH = -\log_{10}(S_{H^+})$

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{64}$ $\quad p_{co2} = S_{gas,co2}\,R\,T$

$p_{h2} = S_{gas,h2}\,\frac{R\,T}{16}$ $\quad p_{gas} = p_{ch4} + p_{co2} + p_{h2} + p_{h2o}$

$q_{gas} = k_p\,(p_{gas}-p_{atm})\,\frac{p_{gas}}{p_{atm}}$

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

Component i →	1	2	3	4	5	6	7	
j Process↓	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	**Process rate ρ_j**
1 Hydrolysis X_{ch}	1.111							$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		1						$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}	0.1348		0.9511					$k_{li}\, X_{li}$
4 Acidogenesis S_{su}	$-\frac{1}{Y_{su}}$				$\frac{0.0763}{Y_{su}} - 0.1013$	$\frac{0.1903}{Y_{su}} - 0.2526$	$\frac{0.4100}{Y_{su}} - 0.5442$	$\mu_{m,su}\, \frac{S_{su}}{K_{S,su} + S_{su}}\, X_{su}\, I_{su}$
5 Acidogenesis S_{aa}		$-\frac{1}{Y_{aa}}$		$\frac{0.1726}{Y_{aa}} - 0.1597$	$\frac{0.2189}{Y_{aa}} - 0.2025$	$\frac{0.0505}{Y_{aa}} - 0.0468$	$\frac{0.5737}{Y_{aa}} - 0.5398$	$\mu_{m,aa}\, \frac{S_{aa}}{K_{S,aa} + S_{aa}}\, X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}			$-\frac{1}{Y_{fa}}$				$\frac{1.8852}{Y_{fa}} - 0.9291$	$\mu_{m,fa}\, \frac{S_{fa}}{K_{S,fa} + S_{fa}}\, X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}				$-\frac{1}{Y_{va}}$		$\frac{0.7274}{Y_{va}} - 0.5052$	$\frac{0.5924}{Y_{va}} - 0.4114$	$\mu_{m,va}\, \frac{S_{va}}{K_{S,va} + S_{va}}\, \frac{X_{va}\, S_{va}}{S_{va} + S_{bu}}\, I_{va}$
8 Acetogenesis S_{bu}					$-\frac{1}{Y_{bu}}$		$\frac{1.3632}{Y_{bu}} - 1.0618$	$\mu_{m,bu}\, \frac{S_{bu}}{K_{S,bu} + S_{bu}}\, \frac{X_{bu}\, S_{bu}}{S_{bu} + S_{va}}\, I_{bu}$
9 Acetogenesis S_{pro}						$-\frac{1}{Y_{pro}}$	$\frac{0.8086}{Y_{pro}} - 0.7565$	$\mu_{m,pro}\, \frac{S_{pro}}{K_{S,pro} + S_{pro}}\, X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}							$-\frac{1}{Y_{ac}}$	$\mu_{m,ac}\, \frac{S_{ac}}{K_{S,ac} + S_{ac}}\, X_{ac}\, I_{ac}$
11 Methanogenesis S_{h2}								$\mu_{m,h2}\, \frac{S_{h2}}{K_{S,h2} + S_{h2}}\, X_{h2}\, I_{h2}$
12 Decay X_{su}								$k_{dec}\, X_{su}$
13 Decay X_{aa}								$k_{dec}\, X_{aa}$
14 Decay X_{fa}								$k_{dec}\, X_{fa}$
15 Decay X_{va}								$k_{dec}\, X_{va}$
16 Decay X_{bu}								$k_{dec}\, X_{bu}$
17 Decay X_{pro}								$k_{dec}\, X_{pro}$
18 Decay X_{ac}								$k_{dec}\, X_{ac}$
19 Decay X_{h2}								$k_{dec}\, X_{h2}$

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

Component i →	8	9	10	11	12	
j Process↓	S_{h2}	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	**Process rate ρ_j**
1 Hydrolysis X_{ch}						$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}						$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}			-0.0293			$k_{li}\, X_{li}$
4 Acidogenesis S_{su}	$\frac{0.0255}{Y_{su}} - 0.0339$		$\frac{0.3731}{Y_{su}} - 0.4977$	-0.1506	$-\frac{0.0753}{Y_{su}} + 0.5777$	$\mu_{m,su} \frac{S_{su}}{K_{S,su} + S_{su}} X_{su}\, I_{su}$
5 Acidogenesis S_{aa}	$\frac{0.0116}{Y_{aa}} - 0.0107$		$\frac{0.2739}{Y_{aa}} - 0.3350$	$\frac{0.1949}{Y_{aa}} - 0.1506$	$-\frac{0.4962}{Y_{aa}} + 0.4362$	$\mu_{m,aa} \frac{S_{aa}}{K_{S,aa} + S_{aa}} X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}	$\frac{0.1085}{Y_{fa}} - 0.0535$		$-\frac{0.0172}{Y_{fa}} - 0.5836$	-0.1506	$-\frac{0.9766}{Y_{fa}} + 0.7167$	$\mu_{m,fa} \frac{S_{fa}}{K_{S,fa} + S_{fa}} X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}	$\frac{0.0385}{Y_{va}} - 0.0267$		$-\frac{0.0102}{Y_{va}} - 0.4419$	-0.1506	$-\frac{0.3481}{Y_{va}} + 0.5358$	$\mu_{m,va} \frac{S_{va}}{K_{S,va} + S_{va}} \frac{X_{va}\, S_{va}}{S_{va} + S_{bu}} I_{va}$
8 Acetogenesis S_{bu}	$\frac{0.0458}{Y_{bu}} - 0.0356$		-0.3891	-0.1506	$-\frac{0.4089}{Y_{bu}} + 0.6371$	$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu} + S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu} + S_{va}} I_{bu}$
9 Acetogenesis S_{pro}	$\frac{0.0819}{Y_{pro}} - 0.0766$		$\frac{0.5971}{Y_{pro}} - 0.8365$	-0.1506	$-\frac{0.4876}{Y_{pro}} + 0.8202$	$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro} + S_{pro}} X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}		$\frac{0.2671}{Y_{ac}} - 0.3546$	$\frac{0.7329}{Y_{ac}} - 0.9727$	-0.1506	0.4778	$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac} + S_{ac}} X_{ac}\, I_{ac}$
11 Methanogenesis S_{h2}	$-\frac{1}{Y_{h2}}$	$\frac{1.9895}{Y_{h2}} - 0.3546$	$-\frac{5.4579}{Y_{h2}} - 0.9727$	-0.1506	$\frac{4.4683}{Y_{h2}} + 0.4778$	$\mu_{m,h2} \frac{S_{h2}}{K_{S,h2} + S_{h2}} X_{h2}\, I_{h2}$
12 Decay X_{su}						$k_{dec}\, X_{su}$
13 Decay X_{aa}						$k_{dec}\, X_{aa}$
14 Decay X_{fa}						$k_{dec}\, X_{fa}$
15 Decay X_{va}						$k_{dec}\, X_{va}$
16 Decay X_{bu}						$k_{dec}\, X_{bu}$
17 Decay X_{pro}						$k_{dec}\, X_{pro}$
18 Decay X_{ac}						$k_{dec}\, X_{ac}$
19 Decay X_{h2}						$k_{dec}\, X_{h2}$

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

Component i →	13	14	15	16	17	18	19	20	21	22	23	
j Process↓	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{va}	X_{bu}	X_{pro}	X_{ac}	X_{h2}	**Process rate ρ_j**
1 Hydrolysis X_{ch}	-1											$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		-1										$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}			-1									$k_{li}\, X_{li}$
4 Acidogenesis S_{su}				1								$\mu_{m,su}\, \frac{S_{su}}{K_{S,su}+S_{su}}\, X_{su}\, I_{su}$
5 Acidogenesis S_{aa}					1							$\mu_{m,aa}\, \frac{S_{aa}}{K_{S,aa}+S_{aa}}\, X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}						1						$\mu_{m,fa}\, \frac{S_{fa}}{K_{S,fa}+S_{fa}}\, X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}							1					$\mu_{m,va}\, \frac{S_{va}}{K_{S,va}+S_{va}}\, \frac{X_{va}\, S_{va}}{S_{va}+S_{bu}}\, I_{va}$
8 Acetogenesis S_{bu}								1				$\mu_{m,bu}\, \frac{S_{bu}}{K_{S,bu}+S_{bu}}\, \frac{X_{bu}\, S_{bu}}{S_{bu}+S_{va}}\, I_{bu}$
9 Acetogenesis S_{pro}									1			$\mu_{m,pro}\, \frac{S_{pro}}{K_{S,pro}+S_{pro}}\, X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}										1		$\mu_{m,ac}\, \frac{S_{ac}}{K_{S,ac}+S_{ac}}\, X_{ac}\, I_{ac}$
11 Methanogenesis S_{h2}											1	$\mu_{m,h2}\, \frac{S_{h2}}{K_{S,h2}+S_{h2}}\, X_{h2}\, I_{h2}$
12 Decay X_{su}	0.18	0.77	0.05	-1								$k_{dec}\, X_{su}$
13 Decay X_{aa}	0.18	0.77	0.05		-1							$k_{dec}\, X_{aa}$
14 Decay X_{fa}	0.18	0.77	0.05			-1						$k_{dec}\, X_{fa}$
15 Decay X_{va}	0.18	0.77	0.05				-1					$k_{dec}\, X_{va}$
16 Decay X_{bu}	0.18	0.77	0.05					-1				$k_{dec}\, X_{bu}$
17 Decay X_{pro}	0.18	0.77	0.05						-1			$k_{dec}\, X_{pro}$
18 Decay X_{ac}	0.18	0.77	0.05							-1		$k_{dec}\, X_{ac}$
19 Decay X_{h2}	0.18	0.77	0.05								-1	$k_{dec}\, X_{h2}$

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

Component i → **j Process↓**	8 S_{h2}	9 S_{ch4}	10 S_{IC}	...	24 S_{an^-}	25 S_{cat^+}	26 S_{va^-}	27 S_{bu^-}	28 S_{pro^-}	29 S_{ac^-}	30 S_{hco3^-}	31 S_{nh3}	32 $S_{gas,h2}$	33 $S_{gas,ch4}$	34 $S_{gas,co2}$	**Process rate** ρ_j
20 Dissociation S_{va}							-1									$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+})-K_{a,va}\,S_{va})$
21 Dissociation S_{bu}								-1								$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+})-K_{a,bu}\,S_{bu})$
22 Dissociation S_{pro}									-1							$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+})-K_{a,pro}\,S_{pro})$
23 Dissociation S_{ac}										-1						$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+})-K_{a,ac}\,S_{ac})$
24 Dissociation S_{IC}											-1					$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+})-K_{a,co2}\,S_{IC})$
25 Dissociation S_{IN}												-1				$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+})-K_{a,IN}\,S_{IN})$
26 Phase transition S_{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{La}\,(S_{h2}-2\,K_{H,h2}\,p_{h2})$
27 Phase transition S_{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4}-16\,K_{H,ch4}\,p_{ch4})$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2}-44\,K_{H,co2}\,p_{co2})$

Inhibition

$I_{su} = I_{aa} = I_{pH,aa}\,I_{IN,lim}$ $\quad I_{fa} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,fa}$ $\quad I_{va} = I_{bu} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,c4}$

$I_{pro} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,pro}$ $\quad I_{ac} = I_{pH,ac}\,I_{IN,lim}\,I_{nh3}$ $\quad I_{h2} = I_{pH,h2}\,I_{IN,lim}$

$$I_{IN,lim} = \frac{S_{IN}}{S_{IN}+K_{S,IN}} \qquad I_{h2,fa} = \frac{K_{I,h2,fa}}{K_{I,h2,fa}+S_{h2}} \qquad I_{h2,c4} = \frac{K_{I,h2,c4}}{K_{I,h2,c4}+S_{h2}}$$

$$I_{h2,pro} = \frac{K_{I,h2,pro}}{K_{I,h2,pro}+S_{h2}} \qquad I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3}+S_{nh3}}$$

$$I_{pH,aa} = \frac{K_{pH,aa}^{n_{aa}}}{K_{pH,aa}^{n_{aa}}+S_{H^+}^{n_{aa}}} \qquad n_{aa} = \frac{3}{pH_{UL,aa}-pH_{LL,aa}} \qquad K_{pH,aa} = 10^{-\frac{pH_{UL,aa}+pH_{LL,aa}}{2}}$$

$$I_{pH,ac} = \frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}}+S_{H^+}^{n_{ac}}} \qquad n_{ac} = \frac{3}{pH_{UL,ac}-pH_{LL,ac}} \qquad K_{pH,ac} = 10^{-\frac{pH_{UL,ac}+pH_{LL,ac}}{2}}$$

$$I_{pH,h2} = \frac{K_{pH,h2}^{n_{h2}}}{K_{pH,aa}^{n_{h2}}+S_{H^+}^{n_{h2}}} \qquad n_{h2} = \frac{3}{pH_{UL,h2}-pH_{LL,h2}} \qquad K_{pH,h2} = 10^{-\frac{pH_{UL,h2}+pH_{LL,h2}}{2}}$$

Algebraic equations

$S_{nh4^+} = S_{IN} - S_{nh3}$ $\quad S_{co2} = S_{IC} - S_{hco3^-}$

$$\phi = S_{cat^+} + \frac{S_{nh4^+}}{17} - \frac{S_{hco3^-}}{44} - \frac{S_{ac^-}}{60} + \frac{S_{pro^-}}{74} - \frac{S_{bu^-}}{88} - \frac{S_{va^-}}{102} - S_{an^-}$$

$$S_{H^+} = -\frac{\phi}{2} + \frac{1}{2}\sqrt{\phi^2+4\,K_w} \qquad pH = -\log_{10}(S_{H^+})$$

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{16}$ $\quad p_{co2} = S_{gas,co2}\,\frac{R\,T}{44}$

$p_{h2} = S_{gas,h2}\,\frac{R\,T}{2}$ $\quad p_{gas} = p_{ch4} + p_{co2} + p_{h2} + p_{h2o}$

$q_{gas} = k_p\,(p_{gas} - p_{atm})\,\frac{p_{gas}}{p_{atm}}$

Weinrich, S.; Nelles, M. (2021): Systematic simplification of the Anaerobic Digestion Model No. 1 (ADM1) – Model development and stoichiometric analysis. *Submitted to Bioresource Technology.*

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

Component i →	1	2	3	4	5	6	7	8	9	10	11	12	
j Process↓	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	**Process rate ρ_j**
1 Hydrolysis X_{ch}	1.111											-0.1111	$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		1											$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}	0.1348		0.9511							-0.0293		-0.0566	$k_{li}\, X_{li}$
4 Acidogenesis S_{su}	-13.2724				0.9113	2.2734	4.8975	0.3047		4.4571	-0.1506	-0.4211	$\mu_{m,su} \frac{S_{su}}{K_{S,su}+S_{su}} X_{su}\, I_{su}$
5 Acidogenesis S_{aa}		-11.5665		1.8371	2.3289	0.5380	6.1053	0.1230		2.8335	2.1033	-5.3026	$\mu_{m,aa} \frac{S_{aa}}{K_{S,aa}+S_{aa}} X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}			-8.2136				14.5554	0.8376		-0.7246	-0.1506	-7.3043	$\mu_{m,fa} \frac{S_{fa}}{K_{S,fa}+S_{fa}} X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}				-11.5757		7.9149	6.4459	0.4188		-0.5594	-0.1506	-3.4940	$\mu_{m,va} \frac{S_{va}}{K_{S,va}+S_{va}} \frac{X_{va}\, S_{va}}{S_{va}+S_{bu}} I_{va}$
8 Acetogenesis S_{bu}					-12.9817		16.6347	0.5584		-0.3891	-0.1506	-4.6718	$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu}+S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu}+S_{va}} I_{bu}$
9 Acetogenesis S_{pro}						-23.3892	18.1566	1.8392		13.1283	-0.1506	-10.5843	$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}							-26.5447		6.7367	18.4808	-0.1506	0.4778	$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
11 Methanogenesis S_{h2}								-2.9703	5.5548	-17.1839	-0.1506	13.7499	$\mu_{m,h2} \frac{S_{h2}}{K_{S,h2}+S_{h2}} X_{h2}\, I_{h2}$
12 Decay X_{su}													$k_{dec}\, X_{su}$
13 Decay X_{aa}													$k_{dec}\, X_{aa}$
14 Decay X_{fa}													$k_{dec}\, X_{fa}$
15 Decay X_{va}													$k_{dec}\, X_{va}$
16 Decay X_{bu}													$k_{dec}\, X_{bu}$
17 Decay X_{pro}													$k_{dec}\, X_{pro}$
18 Decay X_{ac}													$k_{dec}\, X_{ac}$
19 Decay X_{h2}													$k_{dec}\, X_{h2}$

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

Component i →	13	14	15	16	17	18	19	20	21	22	23	
j Process↓	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{va}	X_{bu}	X_{pro}	X_{ac}	X_{h2}	**Process rate ρ_j**
1 Hydrolysis X_{ch}	-1											$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		-1										$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}			-1									$k_{li}\, X_{li}$
4 Acidogenesis S_{su}				1								$\mu_{m,su} \frac{S_{su}}{K_{S,su} + S_{su}} X_{su}\, I_{su}$
5 Acidogenesis S_{aa}					1							$\mu_{m,aa} \frac{S_{aa}}{K_{S,aa} + S_{aa}} X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}						1						$\mu_{m,fa} \frac{S_{fa}}{K_{S,fa} + S_{fa}} X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}							1					$\mu_{m,va} \frac{S_{va}}{K_{S,va} + S_{va}} \frac{X_{va}\, S_{va}}{S_{va} + S_{bu}} I_{va}$
8 Acetogenesis S_{bu}								1				$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu} + S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu} + S_{va}} I_{bu}$
9 Acetogenesis S_{pro}									1			$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro} + S_{pro}} X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}										1		$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac} + S_{ac}} X_{ac}\, I_{ac}$
11 Methanogenesis S_{h2}											1	$\mu_{m,h2} \frac{S_{h2}}{K_{S,h2} + S_{h2}} X_{h2}\, I_{h2}$
12 Decay X_{su}	0.18	0.77	0.05	-1								$k_{dec}\, X_{su}$
13 Decay X_{aa}	0.18	0.77	0.05		-1							$k_{dec}\, X_{aa}$
14 Decay X_{fa}	0.18	0.77	0.05			-1						$k_{dec}\, X_{fa}$
15 Decay X_{va}	0.18	0.77	0.05				-1					$k_{dec}\, X_{va}$
16 Decay X_{bu}	0.18	0.77	0.05					-1				$k_{dec}\, X_{bu}$
17 Decay X_{pro}	0.18	0.77	0.05						-1			$k_{dec}\, X_{pro}$
18 Decay X_{ac}	0.18	0.77	0.05							-1		$k_{dec}\, X_{ac}$
19 Decay X_{h2}	0.18	0.77	0.05								-1	$k_{dec}\, X_{h2}$

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

Component i → **j Process↓**	8 S_{h2}	9 S_{ch4}	10 S_{IC}	...	24 S_{an^-}	25 S_{cat^+}	26 S_{va^-}	27 S_{bu^-}	28 S_{pro^-}	29 S_{ac^-}	30 S_{hco3^-}	31 S_{nh3}	32 $S_{gas,h2}$	33 $S_{gas,ch4}$	34 $S_{gas,co2}$	**Process rate** ρ_j
20 Dissociation S_{va}							-1									$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+})-K_{a,va}\,S_{va})$
21 Dissociation S_{bu}								-1								$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+})-K_{a,bu}\,S_{bu})$
22 Dissociation S_{pro}									-1							$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+})-K_{a,pro}\,S_{pro})$
23 Dissociation S_{ac}										-1						$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+})-K_{a,ac}\,S_{ac})$
24 Dissociation S_{IC}											-1					$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+})-K_{a,co2}\,S_{IC})$
25 Dissociation S_{IN}												-1				$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+})-K_{a,IN}\,S_{IN})$
26 Phase transition S_{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{La}\,(S_{h2}-2\,K_{H,h2}\,p_{h2})$
27 Phase transition S_{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4}-16\,K_{H,ch4}\,p_{ch4})$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2}-44\,K_{H,co2}\,p_{co2})$

Inhibition

$I_{su} = I_{aa} = I_{pH,aa}\,I_{IN,lim}$ $\quad I_{fa} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,fa}$ $\quad I_{va} = I_{bu} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,c4}$

$I_{pro} = I_{pH,aa}\,I_{IN,lim}\,I_{h2,pro}$ $\quad I_{ac} = I_{pH,ac}\,I_{IN,lim}\,I_{nh3}$ $\quad I_{h2} = I_{pH,h2}\,I_{IN,lim}$

$$I_{IN,lim} = \frac{S_{IN}}{S_{IN}+K_{S,IN}} \qquad I_{h2,fa} = \frac{K_{I,h2,fa}}{K_{I,h2,fa}+S_{h2}} \qquad I_{h2,c4} = \frac{K_{I,h2,c4}}{K_{I,h2,c4}+S_{h2}}$$

$$I_{h2,pro} = \frac{K_{I,h2,pro}}{K_{I,h2,pro}+S_{h2}} \qquad I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3}+S_{nh3}}$$

$$I_{pH,aa} = \frac{K_{pH,aa}^{n_{aa}}}{K_{pH,aa}^{n_{aa}}+S_{H^+}^{n_{aa}}} \qquad n_{aa} = \frac{3}{pH_{UL,aa}-pH_{LL,aa}} \qquad K_{pH,aa} = 10^{-\frac{pH_{UL,aa}+pH_{LL,aa}}{2}}$$

$$I_{pH,ac} = \frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}}+S_{H^+}^{n_{ac}}} \qquad n_{ac} = \frac{3}{pH_{UL,ac}-pH_{LL,ac}} \qquad K_{pH,ac} = 10^{-\frac{pH_{UL,ac}+pH_{LL,ac}}{2}}$$

$$I_{pH,h2} = \frac{K_{pH,h2}^{n_{h2}}}{K_{pH,aa}^{n_{h2}}+S_{H^+}^{n_{h2}}} \qquad n_{h2} = \frac{3}{pH_{UL,h2}-pH_{LL,h2}} \qquad K_{pH,h2} = 10^{-\frac{pH_{UL,h2}+pH_{LL,h2}}{2}}$$

Algebraic equations

$S_{nh4^+} = S_{IN} - S_{nh3}$ $\quad S_{co2} = S_{IC} - S_{hco3^-}$

$$\phi = S_{cat^+} + \frac{S_{nh4^+}}{17} - \frac{S_{hco3^-}}{44} - \frac{S_{ac^-}}{60} + \frac{S_{pro^-}}{74} - \frac{S_{bu^-}}{88} - \frac{S_{va^-}}{102} - S_{an^-}$$

$$S_{H^+} = -\frac{\phi}{2} + \frac{1}{2}\sqrt{\phi^2+4\,K_w} \qquad pH = -\log_{10}(S_{H^+})$$

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{16}$ $\quad p_{co2} = S_{gas,co2}\,\frac{R\,T}{44}$

$p_{h2} = S_{gas,h2}\,\frac{R\,T}{2}$ $\quad p_{gas} = p_{ch4} + p_{co2} + p_{h2} + p_{h2o}$

$q_{gas} = k_p\,(p_{gas} - p_{atm})\,\frac{p_{gas}}{p_{atm}}$

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Table 1.4a: Model structure of the mass-based ADM1-R1 (Simplification: hydrogenotrophic methanogenesis)

Component i →	1	2	3	4	5	6	7	8	9	10	11	
j Process↓	S_{su}	S_{aa}	S_{fa}	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	**Process rate** ρ_j
1 Hydrolysis X_{ch}	1.111										-0.1111	$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		1										$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}	0.1348		0.9511						-0.0293		-0.0566	$k_{li}\, X_{li}$
4 Acidogenesis S_{su}	-12.0373				0.8265	2.0619	4.4418	0.5169	2.4433	-0.1506	0.8975	$\mu_{m,su} \frac{S_{su}}{K_{S,su}+S_{su}} X_{su}\, I_{su}$
5 Acidogenesis S_{aa}		-11.1067		1,.7640	2.2363	0.5166	5.8626	0.2208	2.0378	2.0137	-4.5451	$\mu_{m,aa} \frac{S_{aa}}{K_{S,aa}+S_{aa}} X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}			-6.4068				11.3536	1.2219	-4.3451	-0.1506	-2.6730	$\mu_{m,fa} \frac{S_{fa}}{K_{S,fa}+S_{fa}} X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}				-10.1452		6.9368	5.6494	0.6864	-2.6138	-0.1506	-1.3630	$\mu_{m,va} \frac{S_{va}}{K_{S,va}+S_{va}} \frac{X_{va}\, S_{va}}{S_{va}+S_{bu}} I_{va}$
8 Acetogenesis S_{bu}					-10.9274		14.0023	0.8790	-3.0468	-0.1506	-1.7566	$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu}+S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu}+S_{va}} I_{bu}$
9 Acetogenesis S_{pro}						-14.4449	11.2133	2.242	1.5366	-0.1506	-1.2786	$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}							-26.5447	6.7367	18.4808	-0.1506	0.4778	$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
11 Decay X_{su}												$k_{dec}\, X_{su}$
12 Decay X_{aa}												$k_{dec}\, X_{aa}$
13 Decay X_{fa}												$k_{dec}\, X_{fa}$
14 Decay X_{va}												$k_{dec}\, X_{va}$
15 Decay X_{bu}												$k_{dec}\, X_{bu}$
16 Decay X_{pro}												$k_{dec}\, X_{pro}$
17 Decay X_{ac}												$k_{dec}\, X_{ac}$

Table 1.4b: Model structure of the mass-based ADM1-R1 (Simplification: hydrogenotrophic methanogenesis)

Component i →	12	13	14	15	16	17	18	19	20	21	
j Process↓	X_{ch}	X_{pr}	X_{li}	X_{su}	X_{aa}	X_{fa}	X_{va}	X_{bu}	X_{pro}	X_{ac}	**Process rate** ρ_j
1 Hydrolysis X_{ch}	-1										$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}		-1									$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}			-1								$k_{li}\, X_{li}$
4 Acidogenesis S_{su}				1							$\mu_{m,su} \frac{S_{su}}{K_{S,su}+S_{su}} X_{su}\, I_{su}$
5 Acidogenesis S_{aa}					1						$\mu_{m,aa} \frac{S_{aa}}{K_{S,aa}+S_{aa}} X_{aa}\, I_{aa}$
6 Acidogenesis S_{fa}						1					$\mu_{m,fa} \frac{S_{fa}}{K_{S,fa}+S_{fa}} X_{fa}\, I_{fa}$
7 Acetogenesis S_{va}							1				$\mu_{m,c4} \frac{S_{va}}{K_{S,va}+S_{va}} \frac{X_{va}\, S_{va}}{S_{va}+S_{bu}} I_{va}$
8 Acetogenesis S_{bu}								1			$\mu_{m,c4} \frac{S_{bu}}{K_{S,bu}+S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu}+S_{va}} I_{bu}$
9 Acetogenesis S_{pro}									1		$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
10 Methanogenesis S_{ac}										1	$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
11 Decay X_{su}	0.18	0.77	0.05	-1							$k_{dec}\, X_{su}$
12 Decay X_{aa}	0.18	0.77	0.05		-1						$k_{dec}\, X_{aa}$
13 Decay X_{fa}	0.18	0.77	0.05			-1					$k_{dec}\, X_{fa}$
14 Decay X_{va}	0.18	0.77	0.05				-1				$k_{dec}\, X_{va}$
15 Decay X_{bu}	0.18	0.77	0.05					-1			$k_{dec}\, X_{bu}$
16 Decay X_{pro}	0.18	0.77	0.05						-1		$k_{dec}\, X_{pro}$
17 Decay X_{ac}	0.18	0.77	0.05							-1	$k_{dec}\, X_{ac}$

Table 1.4c: Model structure of the mass-based ADM1-R1 (Simplification: hydrogenotrophic methanogenesis)

Component i →	8	9	...	22	23	24	25	26	27	28	29	30	31	
j Process↓	S_{ch4}	S_{IC}		S_{an^-}	S_{cat^+}	S_{va^-}	S_{bu^-}	S_{pro^-}	S_{ac^-}	S_{hco3^-}	S_{nh3}	$S_{gas,ch4}$	$S_{gas,co2}$	**Process rate ρ_j**
18 Dissociation S_{va}						-1								$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+})-K_{a,va}\,S_{va})$
19 Dissociation S_{bu}							-1							$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+})-K_{a,bu}\,S_{bu})$
20 Dissociation S_{pro}								-1						$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+})-K_{a,pro}\,S_{pro})$
21 Dissociation S_{ac}									-1					$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+})-K_{a,ac}\,S_{ac})$
22 Dissociation S_{IC}										-1				$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+})-K_{a,co2}\,S_{IC})$
23 Dissociation S_{IN}											-1			$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+})-K_{a,IN}\,S_{IN})$
24 Phase transition S_{ch4}	-1											$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4}-16\,K_{H,ch4}\,p_{ch4})$
25 Phase transition S_{co2}		-1											$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2}-44\,K_{H,co2}\,p_{co2})$

Inhibition

$I_{su}=I_{aa}=I_{pH,aa}\,I_{IN,lim}$ $\quad I_{fa}=I_{pH,aa}\,I_{IN,lim}$ $\quad I_{va}=I_{bu}=I_{pH,aa}\,I_{IN,lim}$

$I_{pro}=I_{pH,aa}\,I_{IN,lim}$ $\quad I_{ac}=I_{pH,ac}\,I_{IN,lim}\,I_{nh3}$

$$I_{IN,lim}=\frac{S_{IN}}{S_{IN}+K_{S,IN}} \qquad I_{nh3}=\frac{K_{I,nh3}}{K_{I,nh3}+S_{nh3}}$$

$$I_{pH,aa}=\frac{K_{pH,aa}^{n_{aa}}}{K_{pH,aa}^{n_{aa}}+S_{H^+}^{n_{aa}}} \qquad n_{aa}=\frac{3}{pH_{UL,aa}-pH_{LL,aa}} \qquad K_{pH,aa}=10^{-\frac{pH_{UL,aa}+pH_{LL,aa}}{2}}$$

$$I_{pH,ac}=\frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}}+S_{H^+}^{n_{ac}}} \qquad n_{ac}=\frac{3}{pH_{UL,ac}-pH_{LL,ac}} \qquad K_{pH,ac}=10^{-\frac{pH_{UL,ac}+pH_{LL,ac}}{2}}$$

Algebraic equations

$S_{nh4^-}=S_{IN}-S_{nh3}$ $\quad S_{co2}=S_{IC}-S_{hco3^-}$

$$\phi=S_{cat^+}+\frac{S_{nh4^+}}{17}-\frac{S_{hco3^-}}{44}-\frac{S_{ac^-}}{60}-\frac{S_{pro^-}}{74}-\frac{S_{bu^-}}{88}-\frac{S_{va^-}}{102}-S_{an^-}$$

$$S_{H^+}=-\frac{\phi}{2}+\frac{1}{2}\sqrt{\phi^2+4\,K_w} \qquad pH=-\log_{10}(S_{H^+})$$

$$p_{ch4}=S_{gas,ch4}\,\frac{R\,T}{16} \qquad p_{co2}=S_{gas,co2}\,\frac{R\,T}{44}$$

$$p_{gas}=p_{ch4}+p_{co2}+p_{h2o} \qquad q_{gas}=k_p\,(p_{gas}-p_{atm})\,\frac{p_{gas}}{p_{atm}}$$

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Table 1.5a: Model structure of the mass-based ADM1-R2 (Simplification: acidogenesis)

Component i →	1	2	3	4	5	6	7	8	9	10	11	12	
j Process↓	S_{va}	S_{bu}	S_{pro}	S_{ac}	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	X_{ch}	X_{pr}	X_{li}	X_{bac}	**Process rate** ρ_j
1 Hydrolysis X_{ch}		0.0763	0.1903	0.4100	0.0477	0.2255	-0.0139	-0.0283	-1			0.0923	$k_{ch}\, X_{ch}$
2 Hydrolysis X_{pr}	0.1588	0.2014	0.0465	0.5278	0.0199	0.1835	0.1813	-0.4092		-1		0.0900	$k_{pr}\, X_{pr}$
3 Hydrolysis X_{li}		0.0093	0.0231	1.7353	0.1872	-0.6470	-0.0240	-0.4434			-1	0.1597	$k_{li}\, X_{li}$
4 Acetogenesis S_{va}	-10.1452		6.9368	5.6494	0.6864	-2.6138	-0.1506	-1.3630					$\mu_{m,va} \frac{S_{va}}{K_{S,va}+S_{va}} \frac{X_{va}\, S_{va}}{S_{va}+S_{bu}} I_{va}$
5 Acetogenesis S_{bu}		-10.9274		14.0023	0.8790	-3.0468	-0.1506	-1.7566					$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu}+S_{bu}} \frac{X_{bu}\, S_{bu}}{S_{bu}+S_{va}} I_{bu}$
6 Acetogenesis S_{pro}			-14.4449	11.2133	2.1242	1.5366	-0.1506	-1.2786					$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
7 Methanogenesis S_{ac}				-26.5447	6.7367	18.4808	-0.1506	0.4778					$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
8 Decay X_{bac}									0.18	0.77	0.05	-1	$k_{dec}\, X_{bac}$
9 Decay X_{va}									0.18	0.77	0.05		$k_{dec}\, X_{va}$
10 Decay X_{bu}									0.18	0.77	0.05		$k_{dec}\, X_{bu}$
11 Decay X_{pro}									0.18	0.77	0.05		$k_{dec}\, X_{pro}$
12 Decay X_{ac}									0.18	0.77	0.05		$k_{dec}\, X_{ac}$
13 Dissociation S_{va}													$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+}) - K_{a,va}\, S_{va})$
14 Dissociation S_{bu}													$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+}) - K_{a,bu}\, S_{bu})$
15 Dissociation S_{pro}													$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+}) - K_{a,pro}\, S_{pro})$
16 Dissociation S_{ac}													$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+}) - K_{a,ac}\, S_{ac})$
17 Dissociation S_{IC}													$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+}) - K_{a,co2}\, S_{IC})$
18 Dissociation S_{IN}													$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+}) - K_{a,IN}\, S_{IN})$
19 Phase transition S_{ch4}					-1								$k_{La}\,(S_{ch4} - 16\, K_{H,ch4}\, p_{ch4})$
20 Phase transition S_{co2}						-1							$k_{La}\,(S_{co2} - 44\, K_{H,co2}\, p_{co2})$

Table 1.5b: Model structure of the mass-based ADM1-R2 (Simplification: acidogenesis)

Component i →	13	14	15	16	17	18	19	20	21	22	23	24	25	26	
j Process↓	X_{va}	X_{bu}	X_{pro}	X_{ac}	S_{an^-}	S_{cat^+}	S_{va^-}	S_{pro^-}	S_{bu^-}	S_{ac^-}	S_{hco3^-}	S_{nh3}	$S_{ch4,gas}$	$S_{co2,gas}$	**Process rate** ρ_j
1 Hydrolysis X_{ch}															$k_{ch} \cdot X_{ch}$
2 Hydrolysis X_{pr}															$k_{pr} \cdot X_{pr}$
3 Hydrolysis X_{li}															$k_{li} \cdot X_{li}$
4 Acetogenesis S_{va}	1														$\mu_{m,va} \frac{S_{va}}{K_{S,va}+S_{va}} \frac{X_{va}\,S_{va}}{S_{va}+S_{bu}} I_{va}$
5 Acetogenesis S_{bu}		1													$\mu_{m,bu} \frac{S_{bu}}{K_{S,bu}+S_{bu}} \frac{X_{bu}\,S_{bu}}{S_{bu}+S_{va}} I_{bu}$
6 Acetogenesis S_{pro}			1												$\mu_{m,pro} \frac{S_{pro}}{K_{S,pro}+S_{pro}} X_{pro}\, I_{pro}$
7 Methanogenesis S_{ac}				1											$\mu_{m,ac} \frac{S_{ac}}{K_{S,ac}+S_{ac}} X_{ac}\, I_{ac}$
8 Decay X_{bac}															$k_{dec}\, X_{bac}$
9 Decay X_{va}	-1														$k_{dec}\, X_{va}$
10 Decay X_{bu}		-1													$k_{dec}\, X_{bu}$
11 Decay X_{pro}			-1												$k_{dec}\, X_{pro}$
12 Decay X_{ac}				-1											$k_{dec}\, X_{ac}$
13 Dissociation S_{va}							-1								$k_{AB,va}\,(S_{va^-}\,(K_{a,va}+S_{H^+}) - K_{a,va}\,S_{va})$
14 Dissociation S_{bu}								-1							$k_{AB,bu}\,(S_{bu^-}\,(K_{a,bu}+S_{H^+}) - K_{a,bu}\,S_{bu})$
15 Dissociation S_{pro}									-1						$k_{AB,pro}\,(S_{pro^-}\,(K_{a,pro}+S_{H^+}) - K_{a,pro}\,S_{pro})$
16 Dissociation S_{ac}										-1					$k_{AB,ac}\,(S_{ac^-}\,(K_{a,ac}+S_{H^+}) - K_{a,ac}\,S_{ac})$
17 Dissociation S_{IC}											-1				$k_{AB,co2}\,(S_{hco3^-}\,(K_{a,co2}+S_{H^+}) - K_{a,co2}\,S_{IC})$
18 Dissociation S_{IN}												-1			$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN}+S_{H^+}) - K_{a,IN}\,S_{IN})$
19 Phase transition S_{ch4}													$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4} - 16\,K_{H,ch4}\,p_{ch4})$
20 Phase transition S_{co2}														$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2} - 44\,K_{H,co2}\,p_{co2})$

Table 1.5c: Model structure of the mass-based ADM1-R2 (Simplification: acidogenesis)

Inhibition

$I_{va} = I_{bu} = I_{pH,aa}\, I_{IN,lim}$ $\quad I_{pro} = I_{pH,aa}\, I_{IN,lim}$ $\quad I_{ac} = I_{pH,ac}\, I_{IN,lim}\, I_{nh3}$

$I_{IN,lim} = \frac{S_{IN}}{S_{IN} + K_{S,IN}}$ $\quad I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3} + S_{nh3}}$

$I_{pH,aa} = \frac{K_{pH,aa}^{n_{aa}}}{K_{pH,aa}^{n_{aa}} + S_{H+}^{n_{aa}}}$ $\quad n_{aa} = \frac{3}{pH_{UL,aa} - pH_{LL,aa}}$ $\quad K_{pH,aa} = 10^{-\frac{pH_{UL,aa} + pH_{LL,aa}}{2}}$

$I_{pH,ac} = \frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}} + S_{H+}^{n_{ac}}}$ $\quad n_{ac} = \frac{3}{pH_{UL,ac} - pH_{LL,ac}}$ $\quad K_{pH,ac} = 10^{-\frac{pH_{UL,ac} + pH_{LL,ac}}{2}}$

Algebraic equations

$S_{nh4+} = S_{IN} - S_{nh3}$ $\quad S_{co2} = S_{IC} - S_{hco3-}$

$\phi = S_{cat+} + \frac{S_{nh4+}}{17} - \frac{S_{hco3-}}{44} - \frac{S_{ac-}}{60} - \frac{S_{pro-}}{74} - \frac{S_{bu-}}{88} - \frac{S_{va-}}{102} - S_{an-}$

$S_{H+} = -\frac{\phi}{2} + \frac{1}{2}\sqrt{\phi^2 + 4\,K_w}$ $\quad pH = -\log_{10}(S_{H+})$

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{16}$ $\quad p_{co2} = S_{gas,co2}\,\frac{R\,T}{44}$

$p_{gas} = p_{ch4} + p_{co2} + p_{h2o}$ $\quad q_{gas} = k_p\,(p_{gas} - p_{atm})\,\frac{p_{gas}}{p_{atm}}$

Table 1.6a: Model structure of the mass-based ADM1-R3 (Simplification: acetogenesis)

Component i →	1	2	3	4	5	6	7	8	9	10	
j Process↓	S_{ac}	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	X_{ch}	X_{pr}	X_{li}	X_{bac}	X_{ac}	**Process rate ρ_j**
1 Fermentation X_{ch}	0.6555	0.0818	0.2245	-0.0169	-0.0574	-1			0.1125		$k_{ch}\, X_{ch}$
2 Fermentation X_{pr}	0.9947	0.0696	0.1029	0.1746	-0.4767		-1		0.1349		$k_{pr}\, X_{pr}$
3 FermentationX_{li}	1.7651	0.1913	-0.6472	-0.0244	-0.4469			-1	0.1621		$k_{li}\, X_{li}$
4 Methanogenesis S_{ac}	-26.5447	6.7367	18.4808	-0.1506	0.4778					1	$\mu_{m,ac}\,\frac{S_{ac}}{K_{S,ac} + S_{ac}}\, X_{ac}\, I_{ac}$
5 Decay X_{bac}						0.18	0.77	0.05	-1		$k_{dec}\, X_{bac}$
6 Decay X_{ac}						0.18	0.77	0.05		-1	$k_{dec}\, X_{ac}$

	2	3	...	11	12	13	14	15	16	17	
	S_{ch4}	S_{IC}		S_{an-}	S_{cat+}	S_{ac-}	S_{hco3-}	S_{nh3}	$S_{ch4,gas}$	$S_{co2,gas}$	
7 Dissociation S_{ac}						-1					$k_{AB,ac}\,(S_{ac-}\,(K_{a,ac} + S_{H+}) - K_{a,ac}\, S_{ac})$
8 Dissociation S_{IC}							-1				$k_{AB,co2}\,(S_{hco3-}\,(K_{a,co2} + S_{H+}) - K_{a,co2}\, S_{IC})$
9 Dissociation S_{IN}								-1			$k_{AB,IN}\,(S_{nh3}\,(K_{a,IN} + S_{H+}) - K_{a,IN}\, S_{IN})$
10 Phase transition S_{ch4}	-1								$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4} - 16\, K_{H,ch4}\, p_{ch4})$
11 Phase transition S_{co2}		-1								$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{co2} - 44\, K_{H,co2}\, p_{co2})$

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Table 1.6b: Model structure of the mass-based ADM1-R3 (Simplification: acetogenesis)

Inhibition

$I_{ac} = I_{pH,ac}\, I_{IN,lim}\, I_{nh3}$

$I_{IN,lim} = \frac{S_{IN}}{S_{IN} + K_{S,IN}}$ $\quad I_{nh3} = \frac{K_{I,nh3}}{K_{I,nh3} + S_{nh3}}$

$I_{pH,ac} = \frac{K_{pH,ac}^{n_{ac}}}{K_{pH,ac}^{n_{ac}} + S_{H+}^{n_{ac}}}$ $\quad n_{ac} = \frac{3}{pH_{UL,ac} - pH_{LL,ac}}$ $\quad K_{pH,ac} = 10^{-\frac{pH_{UL,ac} + pH_{LL,ac}}{2}}$

Algebraic equations

$S_{nh4^+} = S_{IN} - S_{nh3}$ $\quad S_{co2} = S_{IC} - S_{hco3^-}$

$\phi = S_{cat^+} + \frac{S_{nh4^+}}{17} - \frac{S_{hco2^-}}{44} - \frac{S_{ac^-}}{60} - S_{an^-}$

$S_{H^+} = -\frac{\phi}{2} + \frac{1}{2}\sqrt{\phi^2 + 4\,K_w}$ $\quad pH = -\log_{10}(S_{H^+})$

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{16}$ $\quad p_{co2} = S_{gas,co2}\,\frac{R\,T}{44}$

$p_{gas} = p_{ch4} + p_{co2} + p_{h2o}$ $\quad q_{gas} = k_p\,(p_{gas} - p_{atm})\,\frac{p_{gas}}{p_{atm}}$

Table 1.7: Model structure of the mass-based ADM1-R4 (Simplification: acetoclastic methanogenesis)

Component i →	1	2	3	4	5	6	7	8	9	10	
j Process↓	S_{ch4}	S_{IC}	S_{IN}	S_{h2o}	X_{ch}	X_{pr}	X_{li}	X_{bac}	$S_{ch4,gas}$	$S_{co2,gas}$	**Process rate** ρ_j
1 Fermentation X_{ch}	0.2482	0.6809	-0.0207	-0.0456	-1			0.1372			$k_{ch}\,X_{ch}$
2 Fermentation X_{pr}	0.3221	0.7954	0.1689	-0.4588		-1		0.1723			$k_{pr}\,X_{pr}$
3 Fermentation X_{li}	0.6393	0.5817	-0.0344	-0.4152			-1	0.2286			$k_{li}\,X_{li}$
4 Decay X_{bac}					0.18	0.77	0.05	-1			$k_{dec}\,X_{bac}$
5 Phase transition S_{ch4}	-1								$\frac{V_{liq}}{V_{gas}}$		$k_{La}\,(S_{ch4} - 16\,K_{H,ch4}\,p_{ch4})$
6 Phase transition S_{IC}		-1								$\frac{V_{liq}}{V_{gas}}$	$k_{La}\,(S_{IC} - 44\,K_{H,co2}\,p_{co2})$

Algebraic equations

$p_{ch4} = S_{gas,ch4}\,\frac{R\,T}{16}$ $\quad p_{co2} = S_{gas,co2}\,\frac{R\,T}{44}$ $\quad p_{gas} = p_{ch4} + p_{co2} + p_{h2o}$ $\quad q_{gas} = k_p\,(p_{gas} - p_{atm})\,\frac{p_{gas}}{p_{atm}}$

Table 1.8a: Balancing equations and solution of a simplified reaction model

Differential equations

$$\frac{dX_{ch}}{dt} = D\,(X_{ch,in} - X_{ch}) - X_{ch}\,k_{ch} + f_{ch,x}\,X_{bac}\,k_{dec}$$

$$\frac{dX_{pr}}{dt} = D\,(X_{pr,in} - X_{pr}) - X_{pr}\,k_{pr} + f_{pr,x}\,X_{bac}\,k_{dec}$$

$$\frac{dX_{li}}{dt} = D\,(X_{li,in} - X_{li}) - X_{li}\,k_{li} + f_{li,x}\,X_{bac}\,k_{dec}$$

$$\frac{dX_{bac}}{dt} = D\,(X_{bac,in} - X_{bac}) - X_{bac}\,k_{dec} + Y_{ch}\,X_{ch}\,k_{ch} + Y_{pr}\,X_{pr}\,k_{pr} + Y_{li}\,X_{li}\,k_{li}$$

$$\frac{dV_{ch4}}{dt} = V_{liq}\,(v_{ch4,ch}\,X_{ch}\,k_{ch} + v_{ch4,pr}\,X_{pr}\,k_{pr} + v_{ch4,li}\,X_{li}\,k_{li})$$

$$\frac{dV_{co2}}{dt} = V_{liq}\,(v_{co2,ch}\,X_{ch}\,k_{ch} + v_{co2,pr}\,X_{pr}\,k_{pr} + v_{co2,li}\,X_{li}\,k_{li})$$

. . . . . .

$$D = \frac{1}{HRT} = \frac{q_{liq}}{V_{liq}}$$

Implicit solution for steady state conditions | $\frac{dX_i}{dt} = 0$

$$X_{ch} = \frac{D\,X_{ch,in} + f_{ch,x}\,X_{bac}\,k_{dec}}{D + k_{ch}}$$

$$X_{pr} = \frac{D\,X_{pr,in} + f_{pr,x}\,X_{bac}\,k_{dec}}{D + k_{pr}}$$

$$X_{li} = \frac{D\,X_{li,in} + f_{li,x}\,X_{bac}\,k_{dec}}{D + k_{li}}$$

$$X_{bac} = \frac{D\,X_{bac,in} + (Y_{ch}\,X_{ch}\,k_{ch} + Y_{pr}\,X_{pr}\,k_{pr} + Y_{li}\,X_{li}\,k_{li})}{D + k_{dec}}$$

$$\dot{V}_{ch4} = V_{liq}\,(v_{ch4,ch}\,X_{ch}\,k_{ch} + v_{ch4,pr}\,X_{pr}\,k_{pr} + v_{ch4,li}\,X_{li}\,k_{li})$$

$$\dot{V}_{co2} = V_{liq}\,(v_{co2,ch}\,X_{ch}\,k_{ch} + v_{co2,pr}\,X_{pr}\,k_{pr} + v_{co2,li}\,X_{li}\,k_{li})$$

Table 1.8b: Balancing equations and solution of a simplified reaction model

Explicit solution for steady state conditions | $\frac{dX_i}{dt} = 0$

$$X_{ch} = a_1 + \frac{b_1\,(a_1 Y_{ch}\,k_{ch} + a_2 Y_{pr}\,k_{pr} + a_3 Y_{li}\,k_{li})}{D + k_{dec} - b_1 Y_{ch}\,k_{ch} - b_2 Y_{pr}\,k_{pr} - b_3 Y_{li}\,k_{li}}$$

$$X_{pr} = a_2 + \frac{b_2\,(a_1 Y_{ch}\,k_{ch} + a_2 Y_{pr}\,k_{pr} + a_3 Y_{li}\,k_{li})}{D + k_{dec} - b_1 Y_{ch}\,k_{ch} - b_2 Y_{pr}\,k_{pr} - b_3 Y_{li}\,k_{li}}$$

$$X_{li} = a_3 + \frac{b_3\,(a_1 Y_{ch}\,k_{ch} + a_2 Y_{pr}\,k_{pr} + a_3 Y_{li}\,k_{li})}{D + k_{dec} - b_1 Y_{ch}\,k_{ch} - b_2 Y_{pr}\,k_{pr} - b_3 Y_{li}\,k_{li}}$$

$$X_{bac} = \frac{a_1 Y_{ch}\,k_{ch} + a_2 Y_{pr}\,k_{pr} + a_3 Y_{li}\,k_{li}}{D + k_{dec} - b_1 Y_{ch}\,k_{ch} - b_2 Y_{pr}\,k_{pr} - b_3 Y_{li}\,k_{li}}$$

$$a_1 = \frac{D\,X_{ch,in}}{D + k_{ch}} \qquad a_2 = \frac{D\,X_{pr,in}}{D + k_{pr}} \qquad a_3 = \frac{D\,X_{li,in}}{D + k_{li}}$$

$$b_1 = \frac{f_{ch,x}\,k_{dec}}{D + k_{ch}} \qquad b_2 = \frac{f_{pr,x}\,k_{dec}}{D + k_{pr}} \qquad b_3 = \frac{f_{li,x}\,k_{dec}}{D + k_{li}}$$

Biogas potential for complete degradation of decayed microbial biomass

$$V_{ch4} = (X_{ch,in} + c_1 f_{ch,x})\,v_{ch4,ch} + (X_{pr,in} + c_1 f_{pr,x})\,v_{ch4,pr} + (X_{li,in} + c_1 f_{li,x})\,v_{ch4,li}$$

$$V_{co2} = (X_{ch,in} + c_1 f_{ch,x})\,v_{co2,ch} + (X_{pr,in} + c_1 f_{pr,x})\,v_{co2,pr} + (X_{li,in} + c_1 f_{li,x})\,v_{co2,li}$$

$$c_1 = \frac{X_{ch,in}\,Y_{ch} + X_{pr,in}\,Y_{pr} + X_{li,in}\,Y_{li}}{1 - f_{ch,x}\,Y_{ch} - f_{pr,x}\,Y_{pr} - f_{li,x}\,Y_{li}}$$

Stoichiometric yield coefficients [a]

	ADM1	Angelidaki			ADM1	Angelidaki	
Y_{ch}	0.1372	0.1509	[g g^{-1}]	$v_{ch4,ch}$	347	340	[L kg^{-1}]
Y_{pr}	0.1723	0.1241	[g g^{-1}]	$v_{ch4,pr}$	450	333	[L kg^{-1}]
Y_{li}	0.2286	0.1857	[g g^{-1}]	$v_{ch4,li}$	893	920	[L kg^{-1}]
$f_{ch,x}$	0.18	0.18	[g g^{-1}]	$v_{co2,ch}$	347	340	[L kg^{-1}]
$f_{pr,x}$	0.77	0.82	[g g^{-1}]	$v_{co2,pr}$	405	347	[L kg^{-1}]
$f_{li,x}$	0.05	0.00	[g g^{-1}]	$v_{co2,li}$	296	338	[L kg^{-1}]

[a] Derivation of stoichiometric model parameters based on simplified model structures of the ADM1 (Table 1.7) and the characteristic Angelidaki model [2].

References

[1] Rosen, C. ; Jeppsson, U.: *Aspects on ADM1 Implementation within the BSM2 Framework.* Lund University, Lund, 2006

[2] Weinrich, S. ; Nelles, M.: Critical comparison of different model structures for the applied simulation of the anaerobic digestion of agricultural energy crops. In: *Bioresource Technology.* Vol. 178, No. 1 (2015), pp. 306–312