Petersen matrices

Modell structures

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

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Symbols

$a \mid b \mid c$	Universal constants and parameters	
\mathbf{C}	Carbon content	$[\mathrm{mol}\mathrm{C}\mathrm{g}^{-1}\mathrm{COD}]$
COD	Chemical oxygen demand	
D	Dilution rate	$[d^{-1}]$
f	Yield coefficient	$[g g^{-1}] \mid [g COD g^{-1} COD]$
HRT	Hydraulic retention time	[d]
I	Inhibition function	[-]
k	First-order reaction constant	$[d^{-1}]$
K_{a}	Dissociation constant (acid)	$[\mathrm{mol}\mathrm{L}^{\text{-}1}]$
k_{AB}	Kinetic dissociation rate (acid/base)	$[L \text{ mol}^{-1} \text{ d}^{-1}]$
K_{H}	Henry's law constant	$[\operatorname{mol} \operatorname{L}^{\text{-}1} \operatorname{bar}^{\text{-}1}]$
K_{I}	Inhibition constant	$[\operatorname{g}\operatorname{L}^{\text{-}1}] \mid [\operatorname{g}\operatorname{COD}\operatorname{L}^{\text{-}1}] \mid [\operatorname{mol}\operatorname{L}^{\text{-}1}]$
k_{La}	Volumetric mass transfer coefficient	$[d^{-1}]$
k_{m}	Maximum uptake rate (MONOD)	$[g \operatorname{COD} g^{-1} \operatorname{COD} d^{-1}]$
k_{p}	Pipe friction coefficient	$[L bar^{-1} d^{-1}]$
K_{S}	Half-saturation constant (Monod)	$[\operatorname{g} \operatorname{L}^{\text{-}1}] \mid [\operatorname{g} \operatorname{COD} \operatorname{L}^{\text{-}1}] \mid [\operatorname{mol} \operatorname{L}^{\text{-}1}]$
K_{w}	Ionic product (water)	$[\mathrm{mol}\mathrm{L}^{-1}]$
N	Nitrogen content	$[\mathrm{mol}\mathrm{N}\mathrm{g}^{-1}\mathrm{COD}]$
p	Pressure	[bar]
pK_{a}	Negative logarithmic dissociation constant	[-]
$\rm pH_{LL}\mid \rm pH_{UL}$	Lower and upper pH limit	[-]
q	Volume flow at standard conditions (293 K and 1.01325 bar)	$[L d^{-1}]$
R	Ideal gas constant	$[\operatorname{bar} \operatorname{L} \operatorname{mol}^{-1} \operatorname{K}^{-1}]$
S	Soluble or gaseous component (state variable)	$[g L^{\text{-}1}] \mid [g COD L^{\text{-}1}] \mid [mol L^{\text{-}1}]$
T	Temperature	[K]
V	Volume	[L]
V	Stoichiometric biogas or methane potential	$[\mathrm{Lkg^{ ext{-}1}}]$
X	Particulate component (state variable)	$[g L^{\text{-}1}] \mid [g COD L^{\text{-}1}] \mid [mol L^{\text{-}1}]$
Y	Biomass yield coefficient	$[g g^{-1}] \mid [g COD g^{-1} COD]$
_		
μ_{m}	Maximum growth rate (MONOD)	$[d^{-1}]$
ν	Stoichiometric coefficient	$[-] \mid [g \operatorname{COD} L^{-1}]$
ρ	Process rate Reaction rate	$[gL^{-1}d^{-1}] \mid [gCODL^{-1}d^{-1}] \mid [molL^{-1}d^{-1}]$
$ ho_{\mathrm{T}}$	Transfer rate (phase transition)	$[gL^{-1}d^{-1}] \mid [gCODL^{-1}d^{-1}] \mid [molL^{-1}d^{-1}]$

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

 $\begin{array}{ccc} \text{su} & & \text{Sugars} \\ \text{va} & & \text{Valeric acid} \\ \text{X} & & \text{Microorganisms} \end{array}$

 $\begin{array}{ccc} xc & & Particulate \ composites \\ xI & & Particulate \ inerts \end{array}$

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

	1 S _{su}	2 Saa	3 S_{fa}	4 S _{va}	5 S _{bu}	$_{\mathrm{S}_{\mathrm{pro}}}^{6}$	7 S _{ac}	8 S _{h2}	9 S _{ch4}	10 S _{IC}	11 S _{IN}	Process rate ρ_i
1 Disintegration X _c	Osu	Jaa	ыа	Sva	Бы	Брго	Dac	S _{n2}	Ocn4		N _{xc} -f _{pr,xc} N _{aa}	
2 Hydrolysis X _{ch}										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 - $f_{fa,li}$		$f_{\rm fa,li}$							$\text{-}\!\sum C_i\nu_{i,4}$		$k_{li} X_{li}$
5 Acidogenesis $S_{\rm su}$	-1				$(1-Y_{\mathrm{su}})\mathrm{f_{\mathrm{bu,su}}}$	$(1-Y_{\mathrm{su}})\mathrm{f}_{\mathrm{pro,su}}$	$(1-Y_{\mathrm{su}})\mathrm{f}_{\mathrm{ac,su}}$	$(1-Y_{\mathrm{su}})\mathrm{f_{h2,su}}$		$\text{-}\!\sum C_i\nu_{i,5}$	- $Y_{\rm su}$ $N_{\rm bac}$	$k_{\mathrm{m,su}} \frac{S_{\mathrm{su}}}{K_{\mathrm{S,su}} + S_{\mathrm{su}}} X_{\mathrm{su}} I_{\mathrm{su}}$
6 Acidogenesis S_{aa}		-1		$(1\text{-}Y_{aa})\mathrm{f_{va,aa}}$	$(1-Y_{aa}) f_{bu,aa}$	$(1\text{-}Y_{\mathrm{aa}})\mathrm{f}_{\mathrm{pro,aa}}$	$(1\text{-Y}_{\mathrm{aa}})\mathrm{f}_{\mathrm{ac,aa}}$	$(1-Y_{aa})f_{h2,aa}$		$-\!\sum C_i\nu_{i,6}$	$ m N_{aa} ext{-}Y_{aa} m N_{bac}$	$k_{\mathrm{m,aa}}\frac{\mathrm{S_{aa}}}{\mathrm{K_{S,aa}+S_{aa}}}\mathrm{X_{aa}}\mathrm{I_{aa}}$
7 Acidogenesis S_{fa}			-1				$(1-Y_{\rm fa})0,7$	$(1-Y_{fa}) 0, 3$		$-\!\sum C_i\;\nu_{i,7}$	- $Y_{\rm fa}$ $N_{\rm bac}$	$k_{ m m,fa} rac{S_{ m fa}}{K_{ m S,fa} + S_{ m fa}} X_{ m fa} I_{ m fa}$
8 Acetogenesis S _{va}				-1		$(1-Y_{c4}) 0, 54$	$(1-Y_{c4})0,31$	$(1-Y_{c4}) 0, 15$		$\text{-}\!\sum C_i\nu_{i,8}$	$-\mathrm{Y}_{\mathrm{c4}}\mathrm{N}_{\mathrm{bac}}$	$k_{m,c4} \frac{S_{va}}{K_{S,c4} + S_{va}} \frac{X_{c4} S_{va}}{S_{va} + S_{bu}} I_{c4}$
9 Acetogenesis S_{bu}					-1		$(1-Y_{c4}) 0, 8$	$(1-Y_{c4}) 0, 2$		$\text{-}\!\sum C_i\nu_{i,9}$	$\text{-}Y_{c4}\;N_{bac}$	$k_{m,c4} \frac{S_{bu}}{K_{S,c4} + S_{bu}} \frac{X_{c4} S_{bu}}{S_{bu} + S_{va}} I_{c4}$
10 Acetogenesis S_{pro}						-1	$(1-Y_{ m pro})0,57$	$(1-Y_{ m pro}) 0,43$		$\text{-}\!\sum C_i\nu_{i,10}$	- $Y_{ m pro}$ $N_{ m bac}$	$k_{\rm m,pro}\frac{S_{\rm pro}}{K_{\rm S,pro}+S_{\rm pro}}X_{\rm pro}I_{\rm pro}$
11 Methanogenesis S_{ac}							-1		1-Y _{ac}	$\text{-}\!\sum C_i\nu_{i,11}$	$-Y_{ac} N_{bac}$	$k_{\rm m,ac}\frac{S_{\rm ac}}{K_{\rm S,ac}+S_{\rm ac}}X_{\rm ac}I_{\rm ac}$
12 Methanogenesis S_{h2}	2							-1	$1-Y_{h2}$	$\text{-}\!\sum C_i\nu_{i,12}$	$\text{-}Y_{h2} \; N_{bac}$	$k_{\rm m,h2}\frac{S_{\rm h2}}{K_{\rm S,h2}+S_{\rm h2}}X_{\rm h2}I_{\rm h2}$
13 Decay X _{su}										C_{bac} - C_{xc}	$ m N_{bac}$ - $ m N_{xc}$	k _{dec} X _{su}
14 Decay X _{aa}										C_{bac} - C_{xc}	$\rm N_{bac}\text{-}N_{xc}$	$k_{\rm dec}X_{\rm aa}$
15 Decay X_{fa}										C_{bac} - C_{xc}	$\rm N_{bac}\text{-}N_{xc}$	$k_{\rm dec}X_{\rm fa}$
16 Decay X_{c4}										C_{bac} - C_{xc}	$\rm N_{bac}\text{-}N_{xc}$	$k_{\rm dec}X_{\rm c4}$
17 Decay X_{pro}										C_{bac} - C_{xc}	$\rm N_{bac}\text{-}N_{xc}$	$k_{ m dec} X_{ m pro}$
18 Decay X _{ac}										C_{bac} - C_{xc}	$\rm N_{bac}\text{-}N_{xc}$	$k_{ m dec} X_{ m ac}$
19 Decay X_{h2}										$C_{\mathrm{bac}}\text{-}C_{\mathrm{xc}}$	$\rm N_{\rm bac}\text{-}N_{\rm xc}$	$k_{ m dec} X_{ m h2}$

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

$\begin{array}{ll} \textbf{Component i} \rightarrow \\ \textbf{j} & \textbf{Process} \downarrow \end{array}$	12 $S_{\rm I}$	13 X _c	14 $X_{\rm ch}$	$15 m X_{pr}$	16 X_{1i}	$17 m X_{su}$	18 X _{aa}	19 X_{fa}	20 X_{c4}	21 X_{pro}	22 $_{ m X_{ac}}$	$^{23}_{ m X_{h2}}$	24 $X_{\rm I}$	D
· ·						$\Lambda_{ m su}$	Λ_{aa}	Λ_{fa}	Λ_{c4}	Apro	Aac	Λ_{h2}		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											$k_{\rm ch}~X_{\rm ch}$
3 Hydrolysis X_{pr}				-1										$k_{\rm pr} \: X_{\rm pr}$
4 Hydrolysis X _{li}					-1									$k_{li} X_{li}$
5 Acidogenesis S_{su}						$\rm Y_{su}$								$k_{\mathrm{m,su}}\frac{\mathrm{S_{su}}}{\mathrm{K_{S,su}}+\mathrm{S_{su}}}\mathrm{X_{su}}\mathrm{I_{su}}$
6 Acidogenesis S _{aa}							Y_{aa}							$k_{\mathrm{m,aa}}\frac{S_{\mathrm{aa}}}{K_{\mathrm{S,aa}}+S_{\mathrm{aa}}}X_{\mathrm{aa}}I_{\mathrm{aa}}$
7 Acidogenesis S_{fa}								$\rm Y_{fa}$						$k_{m,fa} rac{S_{fa}}{K_{S,fa} + S_{fa}} X_{fa} I_{fa}$
3 Acetogenesis S _{va}									Y_{c4}					$k_{\rm m,c4} \frac{S_{\rm va}}{K_{\rm S,c4} + S_{\rm va}} \frac{X_{\rm c4} S_{\rm va}}{S_{\rm va} + S_{\rm bu}} I$
Acetogenesis $S_{\rm bu}$									Y_{c4}					$k_{\rm m,c4} \frac{S_{\rm bu}}{K_{\rm S,c4} + S_{\rm bu}} \frac{X_{\rm c4} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}}$
10 Acetogenesis S _{pro}										Y_{pro}				$k_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
1 Methanogenesis S_{ac}											Y_{ac}			$k_{\rm m,ac}\frac{S_{\rm ac}}{K_{\rm S,ac}+S_{\rm ac}}X_{\rm ac}I_{\rm ac}$
12 Methanogenesis S _{h2}												$Y_{\rm h2}$		$k_{\rm m,h2}\frac{S_{\rm h2}}{K_{\rm S,h2}+S_{\rm h2}}X_{\rm h2}I_{\rm h2}$
3 Decay X_{su}		1				-1								$k_{ m dec}~X_{ m su}$
4 Decay X _{aa}		1					-1							$k_{\rm dec} X_{\rm aa}$
5 Decay X_{fa}		1						-1						$k_{\rm dec}X_{\rm fa}$
6 Decay X _{c4}		1							-1					$k_{\rm dec} \: X_{\rm c4}$
7 Decay X_{pro}		1								-1				$k_{\rm dec} X_{\rm pro}$
8 Decay X_{ac}		1									-1			$k_{\rm dec} X_{\rm ac}$
9 Decay X _{h2}		1										-1		$k_{ m dec}X_{ m h2}$

						Table	1.1c:]	Model	struct	ure of	the or	iginal	COD-bas	ed ADM1	[1]	
$\begin{array}{ccc} \textbf{Component i} \rightarrow & \\ \textbf{j} & \textbf{Process} \downarrow & \\ \end{array}$	8 S _{h2}	9 S _{ch4}	10 S_{IC}		25 S _{an} -	$^{26}_{\rm S_{cat^+}}$	27 S _{va} -	28 S _{bu} -	29 S _{pro} -	30 S _{ac} -	31 S _{hco3} -	32 S _{nh3}	$\begin{array}{c} 33 \\ S_{\rm gas,h2} \end{array}$	$\begin{array}{c} 34 \\ S_{\rm gas,ch4} \end{array}$	35 $S_{gas,co2}$	Process rate $\rho_{\rm j}$
20 Dissociation S_{va}							-1									$k_{\rm AB,va} \left(S_{\rm va^{\text{-}}} \left(K_{\rm a,va} + S_{\rm H^{+}} \right) - K_{\rm a,va} S_{\rm va} \right)$
21 Dissociation $\rm S_{bu}$								-1								$k_{\rm AB,bu} (S_{\rm bu^{\text{-}}} (K_{\rm a,bu} + S_{\rm H^{\text{+}}}) - K_{\rm a,bu} S_{\rm bu})$
22 Dissociation S_{pro}									-1							$k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro^{\text{-}}}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H^{+}}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right)$
23 Dissociation S_{ac}										-1						$k_{ m AB,ac} \left({ m S}_{ m ac^{-}} \left({ m K}_{ m a,ac} + { m S}_{ m H^{+}} ight) - { m K}_{ m a,ac} \; { m S}_{ m ac} ight)$
24 Dissociation $S_{\rm IC}$											-1					$k_{\rm AB,co2} (S_{\rm hco3^{\text{-}}} (K_{\rm a,co2} + S_{\rm H^{+}}) - K_{\rm a,co2} S_{\rm IC})$
25 Dissociation S_{IN}												-1				$k_{\rm AB,IN} \left(S_{\rm nh3} \left(K_{\rm a,IN} + S_{\rm H^+} \right) - K_{\rm a,IN} S_{\rm IN} \right)$
26 Phase transition S _{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{\rm La} \left(S_{\rm h2} - 16 K_{\rm H,h2} p_{\rm h2} \right)$
27 Phase transition S _{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{\rm La} \left(S_{\rm ch4} - 64 K_{\rm H, ch4} p_{\rm ch4} \right)$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{\rm La} (S_{\rm co2} - K_{\rm H,co2} p_{\rm co2})$
Inhibition													Algebraic	equations		
$I_{\mathrm{su}} = I_{\mathrm{aa}} = I_{\mathrm{pH,aa}} I_{\mathrm{IN,lim}}$		$I_{\mathrm{fa}} = I_{\mathrm{l}}$	$_{ m pH,aa}$ $ m I_{ m I}$	N,lim	$I_{h2,fa}$		$I_{c4} = I$	_{pH,aa} I _I	$_{ m N,lim}$ $ m I_{h2}$	c4		-	$S_{nh4^+} = S_I$	$_{ m IN}-{ m S_{nh3}}$		$S_{\rm co2} = S_{\rm IC} - S_{\rm hco3}$
$I_{\rm pro} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,pro}$		$I_{\rm ac} = I$	$_{ m pH,ac}$ $ m I_{ m I}$	IN,lim	I_{nh3}		$I_{h2} = I_{h2}$	$ m I_{pH,h2}~I_{I}$	N,lim						S	- S _{pro} - S _{bu} - S _{va}
													$\Phi = S_{cat^+}$	$+ S_{nh4^+} - S_{nh4^+}$	$\frac{1}{64}$	$\frac{S_{\rm pro}^2}{1} + \frac{S_{\rm pro}^2}{112} - \frac{S_{\rm bu}^2}{160} - \frac{S_{\rm va}^2}{208} - S_{\rm an}^2$

$I_{\mathrm{su}} = I_{\mathrm{aa}} = I_{\mathrm{pH,aa}} I_{\mathrm{IN,lim}}$	$I_{\rm fa} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,fa}$	$I_{c4} = I_{pH,aa}I_{IN,lim}I_{h2,c4}$
$I_{\rm pro} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,pro}$	$I_{\rm ac} = I_{\rm pH,ac}I_{\rm IN,lim}I_{\rm nh3}$	$I_{\rm h2} = I_{\rm pH,h2}I_{\rm IN,lim}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}}$	$I_{\rm h2,fa} = \frac{K_{\rm I,h2,fa}}{K_{\rm I,h2,fa} + S_{\rm h2}}$	$I_{\rm h2,c4} = \frac{K_{\rm I,h2,c4}}{K_{\rm I,h2,c4} + S_{\rm h2}}$
$I_{\rm h2,pro} = \frac{K_{\rm I,h2,pro}}{K_{\rm I,h2,pro} + S_{\rm h2}}$	$I_{\rm nh3} = \frac{K_{\rm I, nh3}}{K_{\rm I, nh3} + S_{\rm nh3}}$	
$I_{\rm pH,aa} = \frac{K_{\rm pH,aa}^{\rm n_{aa}}}{K_{\rm pH,aa}^{\rm n_{aa}} + S_{\rm H^+}^{\rm n_{aa}}}$	$n_{aa} = \frac{3}{pH_{\mathrm{UL,aa}} - pH_{\mathrm{LL,aa}}}$	$K_{\mathrm{pH,aa}} = 10^{-}\frac{\mathrm{pH_{UL,aa}} + \mathrm{pH_{LL,aa}}}{2}$
$I_{\mathrm{pH,ac}} = \frac{K_{\mathrm{pH,ac}}^{\mathrm{nac}}}{K_{\mathrm{pH,ac}}^{\mathrm{nac}} + S_{\mathrm{H}^+}^{\mathrm{nac}}}$	$n_{\rm ac} = \frac{3}{p H_{\rm UL,ac} - p H_{\rm LL,ac}}$	$K_{\mathrm{pH,ac}} = 10^{-}\frac{\mathrm{pH_{\mathrm{UL,ac}}} + \mathrm{pH_{\mathrm{LL,ac}}}}{2}$
$I_{pH,h2} = \frac{K_{pH,h2}^{n_{h2}}}{K_{pH,aa}^{n_{h2}} + S_{H^+}^{n_{h2}}}$	$n_{\rm h2} = \frac{3}{p H_{\rm UL,h2} - p H_{\rm LL,h2}}$	$K_{\rm pH,h2} = 10^{-} \frac{\rm pH_{\rm UL,h2} + \rm pH_{\rm LL,h2}}{2}$

$$\begin{split} S_{\rm nh4^+} &= S_{\rm IN} - S_{\rm nh3} & S_{\rm co2} = S_{\rm IC} - S_{\rm hco3^-} \\ \varphi &= S_{\rm cat^+} + S_{\rm nh4^+} - S_{\rm hco3^-} - \frac{S_{\rm ac^-}}{64} + \frac{S_{\rm pro^-}}{112} - \frac{S_{\rm bu^-}}{160} - \frac{S_{\rm va^-}}{208} - S_{\rm an^-} \\ S_{\rm H^+} &= -\frac{\varphi}{2} + \frac{1}{2} \sqrt{\varphi^2 + 4\,K_{\rm w}} & {\rm pH} = -{\rm log}_{10}\,(S_{\rm H^+}) \\ \\ p_{\rm ch4} &= S_{\rm gas, ch4}\,\frac{R\,T}{64} & p_{\rm co2} = S_{\rm gas, co2}\,R\,T \\ \\ p_{\rm h2} &= S_{\rm gas, h2}\,\frac{R\,T}{16} & p_{\rm gas} = p_{\rm ch4} + p_{\rm co2} + p_{\rm h2} + p_{\rm h2o} \\ \\ q_{\rm gas} &= k_{\rm p}\,\left(p_{\rm gas} - p_{\rm atm}\right)\,\frac{p_{\rm gas}}{p_{\rm atm}} \end{split}$$

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

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

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

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

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

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

			Table	1.20	d: Mo	del str	ucture	e of th	e mass	-based	l ADM	1 (vari	iable stoic	chiometric	yield co	efficients)
$\begin{array}{l} \textbf{Component i} \rightarrow \\ \textbf{j} \textbf{Process} \downarrow \end{array}$	8 S _{h2}	9 S _{ch4}	10 S_{IC}		24 S _{an} -	$^{25}_{\rm cat^+}$	26 S _{va} -	27 S _{bu} -	28 S _{pro} -	29 S _{ac} -	30 S _{hco3} -	31 S_{nh3}	$\begin{array}{c} 32 \\ S_{\rm gas,h2} \end{array}$	$\begin{array}{c} 33 \\ S_{\rm gas, ch4} \end{array}$	34 $S_{gas,co2}$	Process rate ρ_j
20 Dissociation S _{va}							-1									$k_{\rm AB,va} \left({\rm S_{va^{\text{-}}}} \left({\rm K_{a,va} + S_{H^{+}}} \right) - {\rm K_{a,va}} {\rm S_{va}} \right)$
21 Dissociation $S_{\rm bu}$								-1								$k_{\mathrm{AB,bu}}\left(S_{\mathrm{bu}^{\text{-}}}\left(K_{\mathrm{a,bu}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,bu}}S_{\mathrm{bu}}\right)$
22 Dissociation S_{pro}									-1							$k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro}^{\text{-}}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right)$
23 Dissociation S_{ac}										-1						$k_{\mathrm{AB,ac}}\left(\mathrm{S_{ac^{\text{-}}}}\left(\mathrm{K_{a,ac}}+\mathrm{S_{H^{+}}}\right)-\mathrm{K_{a,ac}}\mathrm{S_{ac}}\right)$
24 Dissociation $S_{\rm IC}$											-1					$k_{\rm AB,co2} (S_{\rm hco3^{\text{-}}} (K_{\rm a,co2} + S_{\rm H^{+}}) - K_{\rm a,co2} S_{\rm IC})$
25 Dissociation S_{IN}												-1				$k_{\mathrm{AB,IN}}\left(S_{\mathrm{nh3}}\left(K_{\mathrm{a,IN}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,IN}}S_{\mathrm{IN}}\right)$
26 Phase transition S _{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{\rm La} \left(S_{\rm h2} - 2 K_{\rm H,h2} p_{\rm h2} \right)$
27 Phase transition S _{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H, ch4} p_{\rm ch4} \right)$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{\rm La} \left(S_{\rm co2} - 44 K_{\rm H,co2} p_{\rm co2} \right)$
Inhibition													Algebraic	equations		
$I_{\mathrm{su}} = I_{\mathrm{aa}} = I_{\mathrm{pH,aa}} I_{\mathrm{IN,lim}}$		$I_{\mathrm{fa}} = I$	$_{ m pH,aa}$ $ m I_{ m I}$	N,lim	$I_{\mathrm{h2,fa}}$		$I_{\mathrm{va}} = I$	$I_{ m bu}=I_{ m p}$	H,aa I _{IN,}	$_{ m lim} { m I_{h2,c}}$	4	-	$S_{nh4^+} = S_I$	$_{ m N}-S_{ m nh3}$		$S_{co2} = S_{IC} - S_{hco3}$
$I_{\mathrm{pro}} = I_{\mathrm{pH,aa}} I_{\mathrm{IN,lim}} I_{\mathrm{h2,pro}}$	D	$I_{\rm ac} = I$	$I_{ m pH,ac}I_{ m I}$	N,lim	I_{nh3}		$I_{h2} = I$	$I_{ m pH,h2}I_{ m I}$	N,lim				 ф — g	S _{nh4} +	S _{hco3} - S	$\frac{S_{\text{pro}^-}}{60} + \frac{S_{\text{pro}^-}}{74} - \frac{S_{\text{bu}^-}}{88} - \frac{S_{\text{va}^-}}{102} - S_{\text{an}^-}$
													$\Psi - S_{cat}$	$-\frac{17}{17}$	44 ($\frac{74}{60} + \frac{74}{74} - \frac{88}{88} - \frac{102}{102} - \frac{3}{102}$

Inhibition			Algebraic equations
$I_{\rm su} = I_{\rm aa} = I_{\rm pH,aa}I_{\rm IN,lim}$	$I_{\rm fa} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,fa}$	$I_{\mathrm{va}} = I_{\mathrm{bu}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}I_{\mathrm{h2,c4}}$	$S_{{ m nh}4^{+}} = S_{{ m IN}} - S_{{ m nh}3}$ $S_{{ m co}2} = S_{{ m IC}} - S_{{ m hco}3^{-}}$
$I_{\mathrm{pro}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}I_{\mathrm{h2,pro}}$	$I_{\rm ac} = I_{\rm pH,ac} I_{\rm IN,lim} I_{\rm nh3} $	$I_{h2} = I_{pH,h2} I_{IN,lim}$	$\phi = S_{\text{cat}^+} + \frac{S_{\text{nh4}^+}}{17} - \frac{S_{\text{hco3}^-}}{44} - \frac{S_{\text{ac}^-}}{60} + \frac{S_{\text{pro}^-}}{74} - \frac{S_{\text{bu}^-}}{88} - \frac{S_{\text{va}^-}}{102} - S_{\text{an}^-}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}} \label{eq:Indian}$	$I_{\rm h2,fa} = \frac{K_{\rm I,h2,fa}}{K_{\rm I,h2,fa} + S_{\rm h2}}$	$I_{\rm h2,c4} = \frac{K_{\rm I,h2,c4}}{K_{\rm I,h2,c4} + S_{\rm h2}}$	$S_{H^+} = -\frac{\varphi}{2} + \frac{1}{2} \sqrt{\varphi^2 + 4 K_w} \qquad pH = -\log_{10} \left(S_{H^+} \right)$
$I_{\rm h2,pro} = \frac{K_{\rm I,h2,pro}}{K_{\rm I,h2,pro} + S_{\rm h2}} \label{eq:Ih2pro}$	$I_{\rm nh3} = \frac{K_{\rm I, nh3}}{K_{\rm I, nh3} + S_{\rm nh3}}$		$p_{ch4} = S_{gas,ch4} \frac{RT}{16}$ $p_{co2} = S_{gas,co2} \frac{RT}{44}$
$I_{\rm pH,aa} = \frac{K_{\rm pH,aa}^{\rm n_{aa}}}{K_{\rm pH,aa}^{\rm n_{aa}} + S_{\rm H^+}^{\rm n_{aa}}}$	$n_{aa} = \frac{3}{pH_{UL,aa} - pH_{LL,aa}}$	$K_{\mathrm{pH,aa}} = 10^{-}\frac{\mathrm{pH_{UL,aa}} + \mathrm{pH_{LL,aa}}}{2}$	$p_{h2} = S_{gas,h2} \frac{RT}{2}$ $p_{gas} = p_{ch4} + p_{co2} + p_{h2} + p_{h2o}$ $q_{gas} = k_p (p_{gas} - p_{atm}) \frac{p_{gas}}{p_{gas}}$
$I_{\mathrm{pH,ac}} = \frac{K_{\mathrm{pH,ac}}^{\mathrm{nac}}}{K_{\mathrm{pH,ac}}^{\mathrm{nac}} + S_{\mathrm{H}^+}^{\mathrm{nac}}}$	$n_{\rm ac} = \frac{3}{pH_{\rm UL,ac} - pH_{\rm LL,ac}}$	$K_{\mathrm{pH,ac}} = 10^{-}\frac{\mathrm{pH_{UL,ac}} + \mathrm{pH_{LL,ac}}}{2}$	$q_{gas} = \kappa_{p} (p_{gas} - p_{atm}) \frac{1}{p_{atm}}$
$I_{\rm pH,h2} = \frac{K_{\rm pH,h2}^{\rm nh2}}{K_{\rm pH,aa}^{\rm nh2} + S_{\rm H^+}^{\rm nh2}}$	$n_{\rm h2} = \frac{3}{pH_{\rm UL,h2}-pH_{\rm LL,h2}} \label{eq:nh2}$	$K_{pH,h2} = 10^{-\frac{pH_{UL,h2} + pH_{LL,h2}}{2}}$	

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

$\begin{array}{c} \textbf{Component i} \rightarrow \\ \textbf{j} \textbf{Process} \downarrow \end{array}$	$1 S_{su}$	2 S _{aa}	$_{ m S_{fa}}$	4 S_{va}	$_{ m S_{bu}}$	$_{\mathrm{S}_{\mathrm{pro}}}^{6}$	7 Sac	8 S _{h2}	9 S_{ch4}	10 S _{IC}	11 S _{IN}	$12 \\ S_{\rm h2o}$	Process rate ρ_j
1 Hydrolysis X _{ch}	1.111											-0.1111	$k_{\rm ch}X_{\rm ch}$
2 Hydrolysis X_{pr}		1											$k_{\rm pr}X_{\rm pr}$
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	$\mu_{\rm m,su}\frac{S_{\rm su}}{K_{\rm S,su}+S_{\rm su}}X_{\rm su}I_{\rm su}$
5 Acidogenesis S _{aa}		-11.5665		1.8371	2.3289	0.5380	6.1053	0.1230		2.8335	2.1033	-5.3026	$\mu_{\mathrm{m,aa}} \frac{S_{\mathrm{aa}}}{K_{\mathrm{S,aa}} + S_{\mathrm{aa}}} X_{\mathrm{aa}} I_{\mathrm{aa}}$
6 Acidogenesis S_{fa}			-8.2136				14.5554	0.8376		-0.7246	-0.1506	-7.3043	$\mu_{\rm m,fa} \frac{S_{\rm fa}}{K_{\rm S,fa} + S_{\rm fa}} X_{\rm fa} I_{\rm fa}$
7 Acetogenesis S _{va}				-11.5757		7.9149	6.4459	0.4188		-0.5594	-0.1506	-3.4940	$\mu_{\rm m,va} \frac{S_{\rm va}}{K_{\rm S,va} + S_{\rm va}} \frac{X_{\rm va} S_{\rm va}}{S_{\rm va} + S_{\rm bu}} I_{\rm va}$
8 Acetogenesis S _{bu}					-12.9817		16.6347	0.5584		-0.3891	-0.1506	-4.6718	$\mu_{\rm m,bu} \frac{S_{\rm bu}}{K_{\rm S,bu} + S_{\rm bu}} \frac{X_{\rm bu} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}} I_{\rm bu}$
9 Acetogenesis S_{pro}						-23.3892	18.1566	1.8392		13.1283	-0.1506	-10.5843	$\mu_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
10 Methanogenesis S_{ac}							-26.5447		6.7367	18.4808	-0.1506	0.4778	$\mu_{\rm m,ac}\frac{S_{\rm ac}}{K_{\rm S,ac}+S_{\rm ac}}X_{\rm ac}I_{\rm ac}$
11 Methanogenesis S_{h2}								-2.9703	5.5548	-17.1839	-0.1506	13.7499	$\mu_{\rm m,h2} \frac{S_{\rm h2}}{K_{\rm S,h2} + S_{\rm h2}} X_{\rm h2} I_{\rm h2}$
12 Decay X_{su}													$k_{ m dec}X_{ m su}$
13 Decay X _{aa}													$k_{\rm dec} X_{\rm aa}$
14 Decay X_{fa}													$k_{\rm dec}X_{\rm fa}$
15 Decay X_{va}													$k_{\rm dec} X_{\rm va}$
16 Decay X_{bu}													$k_{\rm dec}X_{\rm bu}$
17 Decay X_{pro}													$k_{\rm dec}X_{\rm pro}$
18 Decay X _{ac}													$k_{\rm dec}X_{\rm ac}$
19 Decay X _{h2}													$k_{ m dec}X_{ m h2}$

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

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

			Tab	le 1.	3c: M	lodel st	tructu	re of t	he mas	ss-base	ed ADN	II (fix	xed stoichi	iometric y	rield coef	ficients)
$\begin{array}{c} \textbf{Component i} \rightarrow \\ \textbf{j} \textbf{Process} \downarrow \end{array}$	8 S _{h2}	9 S _{ch4}	10 S_{IC}		24 S _{an} -	$^{25}_{\rm cat^+}$	26 S _{va} -	27 S _{bu} -	28 S _{pro} -	29 S _{ac} -	30 S _{hco3} -	31 S _{nh3}	$\begin{array}{c} 32 \\ S_{\rm gas,h2} \end{array}$	33 $S_{gas,ch4}$	34 $S_{gas,co2}$	Process rate ρ_j
20 Dissociation S _{va}							-1									${\rm k_{AB,va}}\left({{\rm S_{va^{\text{-}}}}\left({{\rm K_{a,va}} + {\rm S_{H^{\text{+}}}}} \right) - {\rm K_{a,va}}{\rm S_{va}}} \right)$
21 Dissociation $S_{\rm bu}$								-1								$k_{\rm AB,bu} \left(S_{\rm bu^{-}} \left(K_{\rm a,bu} + S_{\rm H^{+}} \right) - K_{\rm a,bu} S_{\rm bu} \right)$
22 Dissociation S_{pro}									-1							$k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro}^{*}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right)$
23 Dissociation S _{ac}										-1						$k_{\rm AB,ac} (S_{\rm ac} (K_{\rm a,ac} + S_{\rm H^+}) - K_{\rm a,ac} S_{\rm ac})$
24 Dissociation $S_{\rm IC}$											-1					$k_{\rm AB,co2} (S_{\rm hco3^{\text{-}}} (K_{\rm a,co2} + S_{\rm H^{+}}) - K_{\rm a,co2} S_{\rm IC})$
25 Dissociation S_{IN}												-1				$k_{\mathrm{AB,IN}}\left(S_{\mathrm{nh3}}\left(K_{\mathrm{a,IN}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,IN}}S_{\mathrm{IN}}\right)$
26 Phase transition S _{h2}	-1												$\frac{V_{liq}}{V_{gas}}$			$k_{La} \left(S_{h2} - 2 K_{H,h2} p_{h2} \right)$
27 Phase transition S _{ch4}		-1												$\frac{V_{liq}}{V_{gas}}$		$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H,ch4} p_{\rm ch4} \right)$
28 Phase transition S_{co2}			-1												$\frac{V_{liq}}{V_{gas}}$	$k_{\rm La} \left(S_{\rm co2} - 44 K_{\rm H,co2} p_{\rm co2} \right)$
Inhibition													Algebraic	equations		
$I_{\rm su} = I_{\rm aa} = I_{\rm pH,aa}I_{\rm IN,lim}$		$I_{\mathrm{fa}} = I_{\mathrm{j}}$	_{pH,aa} I _I	N,lim	$I_{h2,fa}$	_	$I_{va} = I$	$_{\mathrm{bu}}=\mathrm{I}_{\mathrm{p}}$	$_{ m H,aa}~{ m I_{IN,l}}$	lim I _{h2,c}	4	-	$S_{nh4^+} = S_I$	$_{ m N}-{ m S}_{ m nh3}$	_	$S_{co2} = S_{IC} - S_{hco3}$
$I_{\mathrm{pro}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}I_{\mathrm{h2,pro}}$)	$I_{\rm ac} = I$	$_{ m pH,ac}$ ${ m I_I}$	N,lim	I_{nh3}		$I_{h2} = I$	$_{ m pH,h2} m I_{ m I}$	N,lim				φ = S	$\frac{S_{nh4^{+}}}{+}$	S _{hco3} - S _z	$\frac{ac^2}{co} + \frac{S_{pro^2}}{74} - \frac{S_{bu^2}}{28} - \frac{S_{va^2}}{102} - S_{an^2}$

Inhibition		
$I_{\rm su} = I_{\rm aa} = I_{\rm pH,aa}I_{\rm IN,lim}$	$I_{\rm fa} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,fa}$	$I_{\mathrm{va}} = I_{\mathrm{bu}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}I_{\mathrm{h2,c4}}$
$I_{\rm pro} = I_{\rm pH,aa}I_{\rm IN,lim}I_{\rm h2,pro}$	$I_{\rm ac} = I_{\rm pH,ac}I_{\rm IN,lim}I_{\rm nh3}$	$I_{\rm h2} = I_{\rm pH,h2}I_{\rm IN,lim}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}} \label{eq:Indian}$	$I_{\rm h2,fa} = \frac{K_{\rm I,h2,fa}}{K_{\rm I,h2,fa} + S_{\rm h2}}$	$I_{\rm h2,c4} = \frac{K_{\rm I,h2,c4}}{K_{\rm I,h2,c4} + S_{\rm h2}}$
$I_{\rm h2,pro} = \frac{K_{\rm I,h2,pro}}{K_{\rm I,h2,pro} + S_{\rm h2}} \label{eq:Ih2pro}$	$I_{\rm nh3} = \frac{K_{\rm I,nh3}}{K_{\rm I,nh3} + S_{\rm nh3}}$	
$I_{\rm pH,aa} = \frac{K_{\rm pH,aa}^{\rm n_{aa}}}{K_{\rm pH,aa}^{\rm n_{aa}} + S_{\rm H^+}^{\rm n_{aa}}}$	$n_{aa} = \frac{3}{pH_{UL,aa} - pH_{LL,aa}}$	$K_{\mathrm{pH,aa}} = 10^{-}\frac{\mathrm{pH_{UL,aa}} + \mathrm{pH_{LL,aa}}}{2}$
$I_{\mathrm{pH,ac}} = \frac{K_{\mathrm{pH,ac}}^{\mathrm{nac}}}{K_{\mathrm{pH,ac}}^{\mathrm{nac}} + S_{\mathrm{H}^+}^{\mathrm{nac}}}$	$n_{\rm ac} = \frac{3}{p H_{\rm UL,ac} - p H_{\rm LL,ac}}$	$K_{\mathrm{pH,ac}} = 10^{-} \frac{\mathrm{pH_{UL,ac}} + \mathrm{pH_{LL,ac}}}{2}$
$I_{\rm pH,h2} = \frac{K_{\rm pH,h2}^{\rm nh2}}{K_{\rm pH,aa}^{\rm nh2} + S_{\rm H^+}^{\rm nh2}}$	$n_{\rm h2} = \frac{3}{pH_{\rm UL,h2}-pH_{\rm LL,h2}}$	$K_{\rm pH,h2} = 10^{-} \frac{\rm pH_{\rm UL,h2} + \rm pH_{\rm LL,h2}}{2}$

$$\begin{split} S_{\rm nh4^+} &= S_{\rm IN} - S_{\rm nh3} & S_{\rm co2} = S_{\rm IC} - S_{\rm hco3^-} \\ & + \frac{S_{\rm nh4^+}}{17} - \frac{S_{\rm hco3^-}}{44} - \frac{S_{\rm ac^-}}{60} + \frac{S_{\rm pro^-}}{74} - \frac{S_{\rm bu^-}}{88} - \frac{S_{\rm va^-}}{102} - S_{\rm an^-} \\ & + \frac{\Phi}{2} + \frac{1}{2} \sqrt{\Phi^2 + 4 \, K_w} & pH = -\log_{10} \left(S_{\rm H^+} \right) \\ & + \frac{\Phi}{2} + \frac{1}{2} \sqrt{\Phi^2 + 4 \, K_w} & p_{\rm co2} = S_{\rm gas, co2} \, \frac{R\, T}{44} \\ & + \frac{\Phi}{2} + \frac{\Phi}{2} + \frac{\Phi}{2} + \frac{\Phi}{2} + \frac{\Phi}{2} + \frac{\Phi}{2} \\ & + \frac{\Phi}{2} \\ & + \frac{\Phi}{2} + \frac{\Phi}{2$$

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

$ \begin{array}{c} \textbf{Component i} \rightarrow \\ \textbf{j} \textbf{Process} \downarrow \end{array} $	$_{ m S_{su}}^{ m 1}$	$_{ m S_{aa}}^{ m 2}$	$_{ m S_{fa}}^{ m 3}$	$_{ m S_{va}}^{ m 4}$	$_{ m S_{bu}}$	$_{ m S_{pro}}^{ m 6}$	$_{ m S_{ac}}^{7}$	$_{ m S_{ch4}}^{ m 8}$	9 S_{IC}	10 S_{IN}	11 S_{h2o}	Process rate ρ_i
1 Hydrolysis X _{ch}	1.111	~aa	⊃1a	- Va	~ Bu	~pro	~ac	CH4	SIC .	~IIV	-0.1111	k _{ch} X _{ch}
2 Hydrolysis X _{pr}	1.111	1									0.1111	$k_{ m pr}X_{ m pr}$
3 Hydrolysis X _{li}	0.1348	1	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	$\mu_{\rm m,su} \frac{S_{\rm su}}{K_{\rm S,su} + S_{\rm su}} X_{\rm su} I_{\rm su}$
5 Acidogenesis S _{aa}		-11.1067		1,.7640	2.2363	0.5166	5.8626	0.2208	2.0378	2.0137	-4.5451	$\mu_{\mathrm{m,aa}} \frac{\mathrm{S_{aa}}}{\mathrm{K_{S,aa} + S_{aa}}} \mathrm{X_{aa}} \mathrm{I_{aa}}$
6 Acidogenesis S_{fa}			-6.4068				11.3536	1.2219	-4.3451	-0.1506	-2.6730	$\mu_{\rm m,fa} \frac{\rm S_{fa}}{\rm K_{S,fa} + S_{fa}} X_{\rm fa} I_{\rm fa}$
7 Acetogenesis S _{va}				-10.1452		6.9368	5.6494	0.6864	-2.6138	-0.1506	-1.3630	$\mu_{\rm m,va} \frac{S_{\rm va}}{K_{\rm S,va} + S_{\rm va}} \frac{X_{\rm va} S_{\rm va}}{S_{\rm va} + S_{\rm bu}} I_{\rm va}$
8 Acetogenesis S_{bu}					-10.9274		14.0023	0.8790	-3.0468	-0.1506	-1.7566	$\mu_{\rm m,bu} \frac{S_{\rm bu}}{K_{\rm S,bu} + S_{\rm bu}} \frac{X_{\rm bu} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}} I_{\rm bu}$
9 Acetogenesis S_{pro}						-14.4449	11.2133	2.242	1.5366	-0.1506	-1.2786	$\mu_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
10 Methanogenesis S_{ac}							-26.5447	6.7367	18.4808	-0.1506	0.4778	$\mu_{\mathrm{m,ac}} \frac{S_{\mathrm{ac}}}{K_{\mathrm{S,ac}} + S_{\mathrm{ac}}} X_{\mathrm{ac}} I_{\mathrm{ac}}$
11 Decay X _{su}												$k_{ m dec} X_{ m su}$
12 Decay X _{aa}												$k_{ m dec} \; X_{ m aa}$
13 Decay X_{fa}												$k_{ m dec}~X_{ m fa}$
14 Decay X_{va}												$k_{ m dec}~X_{ m va}$
15 Decay X_{bu}												$k_{ m dec}~X_{ m bu}$
16 Decay X_{pro}												$k_{ m dec} X_{ m pro}$
17 Decay X _{ac}												$k_{ m dec} X_{ m ac}$

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

$\begin{array}{c} \textbf{Component i} \rightarrow \\ \textbf{j} \textbf{Process} \downarrow \end{array}$	$12 \ X_{\rm ch}$	${\rm ^{13}_{X_{pr}}}$	${}^{14}_{ m X_{li}}$	$15 m X_{su}$	16 X _{aa}	$\begin{array}{c} 17 \\ X_{\mathrm{fa}} \end{array}$	18 X _{va}	$\begin{array}{c} 19 \\ X_{\rm bu} \end{array}$	$\begin{array}{c} 20 \\ X_{\rm pro} \end{array}$	$\begin{array}{c} 21 \\ X_{\rm ac} \end{array}$	Process rate $\rho_{\rm j}$
1 Hydrolysis X_{ch}	-1										$k_{\rm ch}~X_{\rm ch}$
2 Hydrolysis X_{pr}		-1									$k_{\rm pr}X_{\rm pr}$
3 Hydrolysis X _{li}			-1								$k_{li} \: X_{li}$
4 Acidogenesis S_{su}				1							$\mu_{\rm m,su}\frac{\rm S_{\rm su}}{\rm K_{\rm S,su}+S_{\rm su}}X_{\rm su}I_{\rm su}$
5 Acidogenesis S _{aa}					1						$\mu_{\mathrm{m,aa}} \frac{S_{\mathrm{aa}}}{K_{\mathrm{S,aa}} + S_{\mathrm{aa}}} X_{\mathrm{aa}} I_{\mathrm{aa}}$
6 Acidogenesis S_{fa}						1					$\mu_{\rm m,fa} \frac{S_{\rm fa}}{K_{\rm S,fa} + S_{\rm fa}} X_{\rm fa} I_{\rm fa}$
7 Acetogenesis S _{va}							1				$\mu_{\rm m,c4} \frac{S_{\rm va}}{K_{\rm S,va} + S_{\rm va}} \frac{X_{\rm va} S_{\rm va}}{S_{\rm va} + S_{\rm bu}} I_{\rm va}$
8 Acetogenesis S_{bu}								1			$\mu_{\rm m,c4} \frac{S_{\rm bu}}{K_{\rm S,bu} + S_{\rm bu}} \frac{X_{\rm bu} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}} I_{\rm bu}$
9 Acetogenesis S_{pro}									1		$\mu_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
10 Methanogenesis S_{ac}										1	$\mu_{\mathrm{m,ac}} \frac{\mathrm{S_{ac}}}{\mathrm{K_{S,ac} + S_{ac}}} \mathrm{X_{ac}} \mathrm{I_{ac}}$
11 Decay X _{su}	0.18	0.77	0.05	-1							$k_{ m dec} X_{ m su}$
12 Decay X _{aa}	0.18	0.77	0.05		-1						$k_{\rm dec} \: X_{\rm aa}$
13 Decay X_{fa}	0.18	0.77	0.05			-1					$k_{ m dec}~X_{ m fa}$
14 Decay X_{va}	0.18	0.77	0.05				-1				$k_{\rm dec} \: X_{\rm va}$
15 Decay X_{bu}	0.18	0.77	0.05					-1			$k_{\rm dec} X_{\rm bu}$
16 Decay X_{pro}	0.18	0.77	0.05						-1		$k_{\rm dec} \: X_{\rm pro}$
17 Decay X _{ac}	0.18	0.77	0.05							-1	$k_{ m dec} \; X_{ m ac}$

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

$\begin{array}{ll} \textbf{Component} \ \mathbf{i} \ \rightarrow \\ \mathbf{j} \ \ \mathbf{Process} \downarrow \end{array}$	$_{ m S_{ch4}}^{ m 8}$	$_{ m S_{IC}}$		$^{22}_{\rm S_{an}\text{-}}$	$^{23}_{\mathrm{cat}^{+}}$	$^{24}_{\rm S_{va}\text{-}}$	$^{25}_{\rm bu^-}$	$_{ m S_{pro}}$ -	$_{ m S_{ac}}^{27}$	28 $_{ m hco3}$ -	$^{29}_{\rm S_{nh3}}$	30 $S_{\rm gas,ch4}$	31 $S_{gas,co2}$	Process rate $\rho_{\rm j}$
18 Dissociation S _{va}						-1								$k_{\rm AB,va} (S_{\rm va^-} (K_{\rm a,va} + S_{\rm H^+}) - K_{\rm a,va} S_{\rm va})$
19 Dissociation S_{bu} 20 Dissociation S_{pro}							-1	-1						$\begin{split} k_{\mathrm{AB,bu}}\left(S_{\mathrm{bu}^{\text{-}}}\left(K_{\mathrm{a,bu}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,bu}}S_{\mathrm{bu}}\right) \\ \\ k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro}^{\text{-}}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right) \end{split}$
21 Dissociation $S_{\rm ac}$									-1					$k_{\mathrm{AB,ac}}\left(S_{\mathrm{ac}^{-}}\left(K_{\mathrm{a,ac}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,ac}}S_{\mathrm{ac}}\right)$
22 Dissociation $S_{\rm IC}$										-1				$k_{\rm AB,co2} \left(S_{\rm hco3^{\text{-}}} \left(K_{\rm a,co2} + S_{\rm H^{+}} \right) - K_{\rm a,co2} S_{\rm IC} \right)$
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											$\frac{\mathrm{V_{liq}}}{\mathrm{V_{gas}}}$		$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H, ch4} p_{\rm ch4} \right)$
25 Phase transition S_{co2}		-1											$\frac{\mathrm{V_{liq}}}{\mathrm{V_{gas}}}$	$k_{La} \left(S_{co2} - 44 K_{H,co2} p_{co2} \right)$
Inhibition											_	Algebraic e	equations	
$I_{\mathrm{su}} = I_{\mathrm{aa}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}$		$I_{\mathrm{fa}} = I_{\mathrm{pl}}$	$_{ m H,aa}$ ${ m I_{II}}$	N,lim		$I_{\rm va} = I_{\rm bu}$	$=I_{\mathrm{pH,aa}}$	$I_{ m IN,lim}$				$S_{\rm nh4^{\text{-}}} = S_{\rm IN}$	$-S_{nh3}$	$S_{\rm co2} = S_{\rm IC} - S_{\rm hco3}$
$I_{\mathrm{pro}} = I_{\mathrm{pH,aa}} I_{\mathrm{IN,lim}}$		$I_{ac} = I_{p}$	H,ac II	N,lim Inha	3							$\phi = S_{cat^+} +$	$\frac{S_{nh4^{+}}}{17} - \frac{S_{h}}{1}$	$\frac{c_{co3}^{-}}{44} - \frac{S_{ac}^{-}}{60} - \frac{S_{pro}^{-}}{74} - \frac{S_{bu}^{-}}{88} - \frac{S_{va}^{-}}{102} - S_{an}^{-}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}} \label{eq:Innlim}$		$I_{nh3} = \frac{1}{1}$	K _{I,nh3}	$+ S_{nh3}$								$S_{H^+} = -\frac{\varphi}{2}$	1.1	11 00 11 00 102
$\begin{split} I_{\rm pH,aa} &= \frac{K_{\rm pH,aa}^{\rm naa}}{K_{\rm pH,aa}^{\rm na} + S_{\rm H}^{\rm naa}} \\ I_{\rm pH,ac} &= \frac{K_{\rm pH,ac}^{\rm nac}}{K_{\rm pH,ac}^{\rm nac} + S_{\rm H}^{\rm nac}} \end{split}$								$\frac{\text{JL}_{,\text{aa}} + \text{pH}}{2}$ $\frac{\text{JL}_{,\text{ac}} + \text{pH}}{2}$				$p_{ch4} = S_{gas,c}$ $p_{gas} = p_{ch4}$		$\begin{aligned} p_{co2} &= S_{\rm gas,co2} \frac{R.T}{44} \\ \\ o &\qquad q_{\rm gas} = k_{\rm p} \left(p_{\rm gas} - p_{\rm atm} \right) \frac{p_{\rm gas}}{p_{\rm atm}} \end{aligned}$
$K_{pH,ac}^{ac} + S_{H^+}^{ac}$		р	$H_{\mathrm{UL,a}}$	$_{ m c}-{ m pH}_{ m LI}$,ac	$\kappa_{\mathrm{pH,ac}} =$: 10							

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

$\begin{array}{c} \textbf{Component} \ \mathbf{i} \ \rightarrow \\ \mathbf{j} \ \ \mathbf{Process} \downarrow \end{array}$	$1 \\ S_{va}$	$_{ m S_{bu}}^2$	$_{ m S_{pro}}^{ m 3}$	$_{\mathrm{S}_{\mathrm{ac}}}^{4}$	$_{ m S_{ch4}}^{ m 5}$	$_{ m S_{IC}}^{ m 6}$	$7 \\ S_{IN}$	8 $S_{\rm h2o}$	$_{ m X_{ch}}^{ m 9}$	$10 \ { m X_{pr}}$	11 X_{li}	$\begin{array}{c} 12 \\ X_{\rm bac} \end{array}$	Process rate $\rho_{\rm j}$
1 Hydrolysis X _{ch}		0.0763	0.1903	0.4100	0.0477	0.2255	-0.0139	-0.0283	-1			0.0923	$k_{\rm ch}~X_{\rm ch}$
$2 \text{Hydrolysis } X_{\mathrm{pr}}$	0.1588	0.2014	0.0465	0.5278	0.0199	0.1835	0.1813	-0.4092		-1		0.0900	$k_{ m pr}X_{ m pr}$
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					$\mu_{\rm m, va} \frac{S_{\rm va}}{K_{\rm S, va} + S_{\rm va}} \frac{X_{\rm va} S_{\rm va}}{S_{\rm va} + S_{\rm bu}} I_{\rm va}$
5 Acetogenesis S_{bu}		-10.9274		14.0023	0.8790	-3.0468	-0.1506	-1.7566					$\mu_{\rm m,bu} \frac{S_{\rm bu}}{K_{\rm S,bu} + S_{\rm bu}} \frac{X_{\rm bu} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}} I_{\rm bu}$
6 Acetogenesis S_{pro}			-14.4449	11.2133	2.1242	1.5366	-0.1506	-1.2786					$\mu_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
7 Methanogenesis S _{ac}				-26.5447	6.7367	18.4808	-0.1506	0.4778					$\mu_{\mathrm{m,ac}} \frac{S_{\mathrm{ac}}}{K_{\mathrm{S,ac}} + S_{\mathrm{ac}}} X_{\mathrm{ac}} I_{\mathrm{ac}}$
8 Decay X _{bac}									0.18	0.77	0.05	-1	$k_{ m dec}X_{ m bac}$
9 Decay X _{va}									0.18	0.77	0.05		$k_{ m dec} X_{ m va}$
10 Decay X_{bu}									0.18	0.77	0.05		$k_{ m dec}X_{ m bu}$
11 Decay X_{pro}									0.18	0.77	0.05		$k_{ m dec} X_{ m pro}$
12 Decay X _{ac}									0.18	0.77	0.05		$k_{\rm dec}X_{\rm ac}$
13 Dissociation S_{va}													$k_{\rm AB,va} \left(S_{\rm va^{\text{-}}} \left(K_{\rm a,va} + S_{\rm H^{+}} \right) - K_{\rm a,va} S_{\rm va} \right)$
14 Dissociation S_{bu}													$k_{\rm AB,bu} \left(S_{\rm bu^{\text{-}}} \left(K_{\rm a,bu} + S_{\rm H^{\text{+}}} \right) - K_{\rm a,bu} S_{\rm bu} \right)$
15 Dissociation $\rm S_{pro}$													$k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro}^{\text{-}}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right)$
16 Dissociation S_{ac}													$k_{\rm AB,ac} (S_{\rm ac^{\text{-}}} (K_{\rm a,ac} + S_{\rm H^{\text{+}}}) - K_{\rm a,ac} S_{\rm ac})$
17 Dissociation S_{IC}													$k_{AB,co2} \left(S_{hco3} - \left(K_{a,co2} + S_{H^+} \right) - K_{a,co2} S_{IC} \right)$
18 Dissociation S_{IN}													$k_{\mathrm{AB,IN}}\left(S_{\mathrm{nh3}}\left(K_{\mathrm{a,IN}}+S_{\mathrm{H^{+}}}\right)-K_{\mathrm{a,IN}}S_{\mathrm{IN}}\right)$
19 Phase transition S_{ch4}					-1								$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H,ch4} p_{\rm ch4} \right)$
20 Phase transition S_{co2}	2					-1							$k_{\rm La} \left(S_{\rm co2} - 44 K_{\rm H,co2} p_{\rm co2} \right)$

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

															, , , , , , , , , , , , , , , , , , ,
$egin{array}{c} ext{Component i} ightarrow \ ext{j} ext{ Process} \downarrow \end{array}$	13 X_{va}	14 $X_{ m bu}$	15 X_{pro}	16 X_{ac}	17 S _{an} -	$^{18}_{\mathrm{cat}^{+}}$	19 S _{va} -	20 S _{pro} -	21 S _{bu} -	22 $_{\mathrm{ac}}$ -	23 S_{hco3}	24 S_{nh3}	25 $S_{ch4,gas}$	$ m _{Co2,gas}$	Process rate ρ_i
•	va		pro	ac	an	~ cat	~ va	~ pro	~ bu	ac	~hco3	~11113	~cn4,gas	~ C02,gas	
1 Hydrolysis X _{ch}															$ m k_{ch} \cdot X_{ch}$
2 Hydrolysis X_{pr}															$k_{ m pr} \cdot X_{ m pr}$
3 Hydrolysis X _{li}															$k_{li} \cdot X_{li}$
$4 Acetogenesis \; S_{va}$	1														$\mu_{\mathrm{m,va}} \frac{S_{\mathrm{va}}}{K_{\mathrm{S,va}} + S_{\mathrm{va}}} \frac{X_{\mathrm{va}} S_{\mathrm{va}}}{S_{\mathrm{va}} + S_{\mathrm{bu}}} I_{\mathrm{va}}$
$_{5}$ Acetogenesis S_{bu}		1													$\mu_{\rm m,bu} \frac{S_{\rm bu}}{K_{\rm S,bu} + S_{\rm bu}} \frac{X_{\rm bu} S_{\rm bu}}{S_{\rm bu} + S_{\rm va}} I_{\rm bu}$
6 Acetogenesis S_{pro}			1												$\mu_{\rm m,pro} \frac{S_{\rm pro}}{K_{\rm S,pro} + S_{\rm pro}} X_{\rm pro} I_{\rm pro}$
7 Methanogenesis S_{ac}				1											$\mu_{\mathrm{m,ac}} \frac{S_{\mathrm{ac}}}{K_{\mathrm{S,ac}} + S_{\mathrm{ac}}} X_{\mathrm{ac}} I_{\mathrm{ac}}$
8 Decay X _{bac}															$k_{ m dec}X_{ m bac}$
9 Decay X_{va}	-1														$k_{\rm dec}X_{\rm va}$
$10~{\rm Decay}~X_{\rm bu}$		-1													$k_{\rm dec}X_{\rm bu}$
11 Decay X_{pro}			-1												$k_{\rm dec}X_{\rm pro}$
12 Decay X _{ac}				-1											$k_{ m dec}X_{ m ac}$
13 Dissociation S_{va}							-1								$k_{AB,va} (S_{va}^- (K_{a,va} + S_{H^+}) - K_{a,va} S_{va})$
14 Dissociation $S_{\rm bu}$								-1							$k_{\rm AB,bu} (S_{\rm bu^{\text{-}}} (K_{\rm a,bu} + S_{\rm H^{\text{+}}}) - K_{\rm a,bu} S_{\rm bu})$
15 Dissociation S_{pro}									-1						$k_{\mathrm{AB,pro}}\left(S_{\mathrm{pro}^{\text{-}}}\left(K_{\mathrm{a,pro}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,pro}}S_{\mathrm{pro}}\right)$
16 Dissociation S_{ac}										-1					$k_{\rm AB,ac} (S_{\rm ac} (K_{\rm a,ac} + S_{\rm H^+}) - K_{\rm a,ac} S_{\rm ac})$
17 Dissociation $S_{\rm IC}$											-1				$k_{\rm AB,co2} (S_{\rm hco3^{\text{-}}} (K_{\rm a,co2} + S_{\rm H^{\text{+}}}) - K_{\rm a,co2} S_{\rm IC})$
18 Dissociation $S_{\rm IN}$												-1			$k_{\mathrm{AB,IN}}\left(S_{\mathrm{nh3}}\left(K_{\mathrm{a,IN}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,IN}}S_{\mathrm{IN}}\right)$
19 Phase transition S_{ch4}													$\frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}}$		$k_{\rm La} \left({\rm S_{ch4} - 16K_{H,ch4}p_{ch4}} \right)$
20 Phase transition S_{co2}														$\frac{V_{liq}}{V_{gas}}$	$k_{\rm La} (S_{\rm co2} - 44 K_{\rm H,co2} p_{\rm co2})$

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

Inhibition			Algebraic equations	
$I_{\mathrm{va}} = I_{\mathrm{bu}} = I_{\mathrm{pH,aa}}I_{\mathrm{IN,lim}}$	$I_{\rm pro} = I_{\rm pH,aa}I_{\rm IN,lim}$	$I_{\rm ac} = I_{\rm pH,ac}I_{\rm IN,lim}I_{\rm nh3}$	$S_{\rm nh4^+} = S_{\rm IN} - S_{\rm nh3}$	$S_{\rm co2} = S_{\rm IC} - S_{\rm hco3}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}}$	$I_{\rm nh3} = \frac{K_{\rm I, nh3}}{K_{\rm I, nh3} + S_{\rm nh3}}$		$\phi = S_{cat^{+}} + \frac{S_{nh4^{+}}}{17} - \frac{S_{hco3^{-}}}{44} - \frac{S_{cat^{-}}}{6}$	$\frac{S_{\text{pro}}}{0} - \frac{S_{\text{pro}}}{74} - \frac{S_{\text{bu}}}{88} - \frac{S_{\text{va}}}{102} - S_{\text{an}}$
$I_{\mathrm{pH,aa}} = \frac{K_{\mathrm{pH,aa}}^{\mathrm{naa}}}{K_{\mathrm{pH,aa}}^{\mathrm{naa}} + S_{\mathrm{H}+}^{\mathrm{naa}}}$	$n_{aa} = \frac{3}{pH_{UL,aa} - pH_{LL,aa}}$	$\mathrm{K_{pH,aa}=10}^{-}\frac{\mathrm{pH_{UL,aa}+pH_{LL,aa}}}{2}$	$S_{H^{+}} = -\frac{\varphi}{2} + \frac{1}{2}\sqrt{\varphi^{2} + 4K_{w}}$	$pH = -\log_{10}\left(S_{H^+}\right)$
$I_{\mathrm{pH,ac}} = \frac{K_{\mathrm{pH,ac}}^{\mathrm{nac}}}{K_{\mathrm{pH,ac}}^{\mathrm{nac}} + S_{\mathrm{H}^+}^{\mathrm{nac}}}$	$n_{\rm ac} = \frac{3}{p H_{\rm UL,ac} - p H_{\rm LL,ac}}$	$K_{\mathrm{pH,ac}} = 10^{-}\frac{\mathrm{pH_{UL,ac}} + \mathrm{pH_{LL,ac}}}{2}$	$p_{ch4} = S_{gas,ch4} \frac{RT}{16}$ $p_{gas} = p_{ch4} + p_{co2} + p_{h2o}$	$egin{aligned} & p_{\mathrm{co2}} = S_{\mathrm{gas,co2}} rac{R T}{44} \ & \ & \ & \ & \ & \ & \ & \ & \ & \ $

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

${\bf Component} {\bf i} \rightarrow $	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		$k_{\mathrm{ch}}~X_{\mathrm{ch}}$
$2 \text{Fermentation } X_{\rm pr}$	0.9947	0.0696	0.1029	0.1746	-0.4767		-1		0.1349		$k_{ m pr}~X_{ m pr}$
$3 Fermentation X_{li} \\$	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	$\mu_{\mathrm{m,ac}} \frac{S_{\mathrm{ac}}}{K_{\mathrm{S,ac}} + S_{\mathrm{ac}}} X_{\mathrm{ac}} I_{\mathrm{ac}}$
5 Decay X _{bac}						0.18	0.77	0.05	-1		$k_{ m dec}X_{ m bac}$
6 Decay X _{ac}						0.18	0.77	0.05		-1	$k_{ m dec}X_{ m ac}$
	$_{\rm S_{ch4}}^{2}$	$_{ m S_{IC}}^{ m 3}$		11 S _{an} -	$^{12}_{\mathrm{S}_{\mathrm{cat}^{+}}}$	13 S _{ac} -	$^{14}_{ m hco3}$ -	$^{15}_{\mathrm{nh3}}$	16 $S_{ch4,gas}$	$\begin{array}{c} 17 \\ S_{\rm co2,gas} \end{array}$	
7 Dissociation S _{ac}						-1					$k_{ m AB,ac} (S_{ m ac}^{-} (K_{ m a,ac} + S_{ m H^+}) - K_{ m a,ac} S_{ m ac})$
8 Dissociation $S_{\rm IC}$							-1				$k_{\rm AB,co2} (S_{\rm hco3^{\text{-}}} (K_{\rm a,co2} + S_{\rm H^{\text{+}}}) - K_{\rm a,co2} S_{\rm IC})$
9 Dissociation S_{IN}								-1			$k_{\mathrm{AB,IN}}\left(S_{\mathrm{nh3}}\left(K_{\mathrm{a,IN}}+S_{\mathrm{H}^{+}}\right)-K_{\mathrm{a,IN}}S_{\mathrm{IN}}\right)$
10 Phase transition S_{ch4}	-1								$\frac{V_{\mathrm{liq}}}{V_{\mathrm{gas}}}$		$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H,ch4} p_{\rm ch4} \right)$
11 Phase transition S_{co2}		-1								$\frac{\mathrm{V_{liq}}}{\mathrm{V_{gas}}}$	$k_{\rm La} \left(S_{\rm co2} - 44 K_{\rm H,co2} p_{\rm co2} \right)$

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

Inhibition				Algebraic equations	
$I_{\rm ac} = I_{\rm pH,ac}I_{\rm IN,lim}I_{\rm nh3}$				$S_{\rm nh4^+} = S_{\rm IN} - S_{\rm nh3}$	$S_{\rm co2} = S_{\rm IC} - S_{\rm hco3}$
$I_{\rm IN,lim} = \frac{S_{\rm IN}}{S_{\rm IN} + K_{\rm S,IN}}$	$I_{\rm nh3} = \frac{K_{\rm I,nh3}}{K_{\rm I,nh3} + S_{\rm nh3}}$		•••	$\phi = S_{cat^{+}} + \frac{S_{nh4^{+}}}{17} - \frac{S_{hco2^{-}}}{44} - \frac{S_{hco2^{-}}}{44}$	$\frac{S_{ac^-}}{60} - S_{an^-}$
$I_{\rm pH,ac} = \frac{K_{\rm pH,ac}^{\rm nac}}{K_{\rm pH,ac}^{\rm nac} + S_{\rm rel}^{\rm nac}}$	$n_{ac} = \frac{3}{pH_{UL,ac} - pH_{LL,ac}}$	$K_{\mathrm{pH,ac}} = 10 - \frac{\mathrm{pH_{UL,ac}} + \mathrm{pH_{LL,ac}}}{2}$	•••	$S_{H^+} = -\frac{\varphi}{2} + \frac{1}{2} \sqrt{\varphi^2 + 4 K_w}$	$pH = -log_{10}\left(S_{H^+}\right)$
pir,ac HT	, , ,			$p_{\mathrm{ch4}} = S_{\mathrm{gas,ch4}} \tfrac{\mathrm{R} \mathrm{T}}{16}$	$p_{co2} = S_{gas,co2} \frac{R.T}{44}$
				$p_{\rm gas} = p_{\rm ch4} + p_{\rm co2} + p_{\rm h2o}$	$q_{\rm gas} = k_{\rm p} \ (p_{\rm gas} - p_{\rm atm}) \ \frac{p_{\rm gas}}{p_{\rm atm}}$

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

$\begin{array}{c} \textbf{Component i} \rightarrow \\ \textbf{j Process} \downarrow \end{array}$	$_{ m S_{ch4}}^{ m 1}$	$_{ m S_{IC}}^2$	$_{ m S_{IN}}^{ m 3}$	$^{\rm 4}_{\rm S_{h2o}}$	$_{ m X_{ch}}^{ m 5}$	$^{6}_{\rm X_{pr}}$	$\begin{matrix} 7 \\ X_{1i} \end{matrix}$	$\begin{array}{c} 8 \\ X_{\rm bac} \end{array}$	$_{\rm S_{ch4,gas}}^{9}$	$10 \\ S_{\rm co2,gas}$	Process rate $\rho_{\rm j}$
1 Fermentation X _{ch}	0.2482	0.6809	-0.0207	-0.0456	-1			0.1372			$k_{\mathrm{ch}}~X_{\mathrm{ch}}$
2 Fermentation X_{pr}	0.3221	0.7954	0.1689	-0.4588		-1		0.1723			$k_{ m pr} X_{ m pr}$
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			$k_{ m dec}X_{ m bac}$
5 Phase transition S_{ch4}	-1								$\frac{V_{liq}}{V_{gas}}$		$k_{\rm La} \left(S_{\rm ch4} - 16 K_{\rm H,ch4} p_{\rm ch4} \right)$
6 Phase transition $S_{\rm IC}$		-1								$\frac{V_{liq}}{V_{gas}}$	$k_{\rm La} (S_{\rm IC} - 44 K_{\rm H,co2} p_{\rm co2})$
Algebraic equations											
$p_{ch4} = S_{gas, ch4} \frac{RT}{16}$		p _{co2} =	= S _{gas.co2} RT		p _o	$p_{as} = p_{ch4} + p_{ch4}$	₂₀₂ + p _{h20}		Q _{gas}	= k _p (p _{gas} -	- p _{atm}) <u>pgas</u>

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

Differential equations

$$\begin{split} &\frac{dX_{ch}}{dt} = D\left(X_{ch,in} - X_{ch}\right) - X_{ch}\,k_{ch} + f_{ch,x}\,X_{bac}\,k_{dec} \\ &\frac{dX_{pr}}{dt} = D\left(X_{pr,in} - X_{pr}\right) - X_{pr}\,k_{pr} + f_{pr,x}\,X_{bac}\,k_{dec} \\ &\frac{dX_{li}}{dt} = D\left(X_{li,in} - X_{li}\right) - X_{li}\,k_{li} + f_{li,x}\,X_{bac}\,k_{dec} \\ &\frac{dX_{bac}}{dt} = D\left(X_{bac,in} - X_{bac}\right) - X_{bac}\,k_{dec} + Y_{ch}\,X_{ch}\,k_{ch} + Y_{pr}\,X_{pr}\,k_{pr} + Y_{li}\,X_{li}\,k_{li} \\ &\frac{dV_{ch4}}{dt} = V_{liq}\left(v_{ch4,ch}\,X_{ch}\,k_{ch} + v_{ch4,pr}\,X_{pr}\,k_{pr} + v_{ch4,li}\,X_{li}\,k_{li}\right) \\ &\frac{dV_{co2}}{dt} = V_{liq}\left(v_{co2,ch}\,X_{ch}\,k_{ch} + v_{co2,pr}\,X_{pr}\,k_{pr} + v_{co2,li}\,X_{li}\,k_{li}\right) \\ &D = \frac{1}{HRT} = \frac{q_{1iq}}{V_{liq}} \end{split}$$

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

$$\begin{split} X_{ch} &= \frac{D\,X_{ch,in}\,+\,f_{ch,x}\,X_{bac}\,k_{dec}}{D\,+\,k_{ch}} \\ X_{pr} &= \frac{D\,X_{pr,in}\,+\,f_{pr,x}\,X_{bac}\,k_{dec}}{D\,+\,k_{pr}} \\ X_{li} &= \frac{D\,X_{li,in}\,+\,f_{li,x}\,X_{bac}\,k_{dec}}{D\,+\,k_{li}} \\ X_{bac} &= \frac{D\,X_{bac,in}\,+\,(\,Y_{ch}\,X_{ch}\,k_{ch}\,+\,Y_{pr}\,X_{pr}\,k_{pr}\,+\,Y_{li}\,X_{li}\,k_{li})}{D\,+\,k_{dec}} \\ \dot{V}_{ch4} &= V_{liq}\,(\,v_{ch4,ch}\,X_{ch}\,k_{ch}\,+\,v_{ch4,pr}\,X_{pr}\,k_{pr}\,+\,v_{ch4,li}\,X_{li}\,k_{li}) \\ \dot{V}_{co2} &= V_{liq}\,(\,v_{co2,ch}\,X_{ch}\,k_{ch}\,+\,v_{co2,pr}\,X_{pr}\,k_{pr}\,+\,v_{co2,li}\,X_{li}\,k_{li}) \end{split}$$

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

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

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

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

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

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

$$\begin{split} a_1 &= \frac{D\,X_{\mathrm{ch,in}}}{D\,+\,k_{\mathrm{ch}}} & a_2 &= \frac{D\,X_{\mathrm{pr,in}}}{D\,+\,k_{\mathrm{pr}}} & a_3 &= \frac{D\,X_{\mathrm{li,in}}}{D\,+\,k_{\mathrm{li}}} \\ b_1 &= \frac{f_{\mathrm{ch,x}}\,k_{\mathrm{dec}}}{D\,+\,k_{\mathrm{ch}}} & b_2 &= \frac{f_{\mathrm{pr,x}}\,k_{\mathrm{dec}}}{D\,+\,k_{\mathrm{pr}}} & b_3 &= \frac{f_{\mathrm{li,x}}\,k_{\mathrm{dec}}}{D\,+\,k_{\mathrm{li}}} \end{split}$$

Biogas potential for complete degradation of decayed microbial biomass

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

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

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

Stoichiometric yield coefficients^a

	ADM1	Angelidaki		ADM1	Angelidaki
Y_{ch}	0.1372	$0.1509 \ [\mathrm{g}\mathrm{g}^{\text{-1}}]$	$v_{\rm ch4,ch}$	347	$340 \ [{\rm Lkg^{-1}}]$
$\rm Y_{\rm pr}$	0.1723	$0.1241 \ [g g^{-1}]$	$v_{\mathrm{ch4,pr}}$	450	$333 [\mathrm{Lkg^{-1}}]$
Y_{li}	0.2286	$0.1857 \ [\mathrm{g}\mathrm{g}^{\text{-1}}]$	V _{ch4} ,li	893	$920 \ [{ m Lkg^{-1}}]$
$f_{\mathrm{ch,x}}$	0.18	$0.18 \ [\mathrm{g}\mathrm{g}^{\text{-1}}]$	$v_{\rm co2,ch}$	347	$340 \ [{\rm Lkg^{\text{-}1}}]$
$f_{ m pr,x}$	0.77	$0.82 \ [\mathrm{g}\mathrm{g}^{\text{-}1}]$	$v_{\rm co2,pr}$	405	$347 \ [{\rm Lkg^{-1}}]$
$f_{\mathrm{li},\mathbf{x}}$	0.05	$0.00 \ [\mathrm{g}\mathrm{g}^{\text{-1}}]$	$v_{\rm co2,li}$	296	$338 \ [{ m Lkg^{-1}}]$

^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
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