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**Appendix A.1** Biochemical rate coefficients ( $v_{i,j}$ ) and kinetic rate equations ( $\rho_j$ ) for soluble components ( $i = 1 - 12, j = 1 - 19$ )

$j$	Component → Process ↓	$i$	1 $S_{su}$	2 $S_{aa}$	3 $S_{fa}$	4 $S_{va}$	5 $S_{bu}$	6 $S_{pro}$	7 $S_{ac}$	8 $S_{h2}$	9 $S_{ch4}$	10 $S_{ic}$	11 $S_{in}$	12 $S_i$	Rate ( $\rho_j$ , kg COD.m <sup>-3</sup> .d <sup>-1</sup> )
1	Disintegration														$f_{sl,xc}$
2	Hydrolysis carbohydrates		1												$k_{dis}X_c$
3	Hydrolysis of proteins			1											$k_{hyd,ch}X_{ch}$
4	Hydrolysis of lipids		$1-f_{fa,li}$		$1-f_{fa,li}$										$k_{hyd,pr}X_{pr}$ $k_{hyd,li}X_{li}$
5	Uptake of sugars		-1				$(1-Y_{su})f_{bu,su}$	$(1-Y_{su})f_{pro,su}$	$(1-Y_{su})f_{ac,su}$	$(1-Y_{su})f_{h2,su}$		$-\sum_{i=0,11-24} C_i v_{i,5}$	$-(Y_{su})N_{bac}$		$k_{m,su} \frac{S_{su}}{K_S + S} X_{su} / I_1$
6	Uptake of amino acids			-1		$(1-Y_{aa})f_{va,aa}$	$(1-Y_{aa})f_{bu,aa}$	$(1-Y_{aa})f_{pro,aa}$	$(1-Y_{aa})f_{ac,aa}$	$(1-Y_{aa})f_{h2,aa}$		$-\sum_{i=1-9,11-24} C_i v_{i,6}$	$N_{aa} - (Y_{aa})N_{bac}$		$k_{m,aa} \frac{S_{aa}}{K_S + S_{aa}} X_{aa} / I_1$
7	Uptake of LCFA				-1				$(1-Y_{fa})0.7$	$(1-Y_{fa})0.3$			$-(Y_{fa})N_{bac}$		$k_{m,fa} \frac{S_{fa}}{K_S + S_{fa}} X_{fa} / I_2$
8	Uptake of valerate					-1		$(1-Y_{c4})0.54$	$(1-Y_{c4})0.31$	$(1-Y_{c4})0.15$			$-(Y_{c4})N_{bac}$		$k_{m,c4} \frac{S_{c4}}{K_S + S_{c4}} X_{c4} \frac{1}{1 + S_{c4}/S_{su}}$
9	Uptake of butyrate						-1	$(1-Y_{c4})0.8$	$(1-Y_{c4})0.2$				$-(Y_{c4})N_{bac}$		$k_{m,c4} \frac{S_{c4}}{K_S + S_{c4}} X_{c4} \frac{1}{1 + S_{c4}/S_{su}}$
10	Uptake of propionate							$(1-Y_{pro})0.62$	$(1-Y_{pro})0.43$			$-\sum_{i=1-9,11-24} C_i v_{i,10}$	$-(Y_{pro})N_{bac}$		$k_{m,pr} \frac{S_{pro}}{K_S + S_{pro}} X_{pro} / I_2$
11	Uptake of acetate								$(1-Y_{ac})$			$-\sum_{i=1-9,11-24} C_i v_{i,11}$	$-(Y_{ac})N_{bac}$		$k_{m,ac} \frac{S_{ac}}{K_S + S_{ac}} X_{ac} / I_3$
12	Uptake of hydrogen									-1	$(1-Y_{h2})$	$-\sum_{i=1-9,11-24} C_i v_{i,12}$	$-(Y_{h2})N_{bac}$		$k_{m,h2} \frac{S_{h2}}{K_S + S_{h2}} X_{h2} / I_1$
13	Decay of $X_{su}$														$k_{dec,Xsu}X_{su}$
14	Decay of $X_{aa}$														$k_{dec,Xaa}X_{aa}$
15	Decay of $X_{fa}$														$k_{dec,Xfa}X_{fa}$
16	Decay of $X_{c4}$														$k_{dec,Xc4}X_{c4}$
17	Decay of $X_{pro}$														$k_{dec,Xpro}X_{pro}$
18	Decay of $X_{ac}$														$k_{dec,Xac}X_{ac}$
19	Decay of $X_{h2}$														$k_{dec,Xh2}X_{h2}$



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Mono-saccharides  
(kgCOD.m<sup>-3</sup>)

Amino acids  
(kgCOD.m<sup>-3</sup>)

Long chain fatty acids  
(kgCOD.m<sup>-3</sup>)

Total valerate  
(kgCOD.m<sup>-3</sup>)

Total butyrate  
(kgCOD.m<sup>-3</sup>)

Total propionate  
(kgCOD.m<sup>-3</sup>)

Total acetate  
(kgCOD.m<sup>-3</sup>)

Hydrogen gas  
(kgCOD.m<sup>-3</sup>)

Methane gas  
(kgCOD.m<sup>-3</sup>)

Inorganic carbon  
(kmole C.m<sup>-3</sup>)

Inorganic nitrogen  
(kmole N.m<sup>-3</sup>)

Soluble inerts  
(kgCOD.m<sup>-3</sup>)

Inhibition factors:  
 $I_1 = \frac{1}{1 + \frac{S_{su}}{K_{i1}}}$   
 $I_2 = \frac{1}{1 + \frac{S_{fa}}{K_{i2}}}$   
 $I_3 = \frac{1}{1 + \frac{S_{ac}}{K_{i3}}}$

**Appendix A.2** Biochemical rate coefficients ( $v_{i,j}$ ) and kinetic rate equations ( $p_j$ ) for soluble components ( $i = 13 - 24, j = 1 - 19$ )

$j$	Component → Process ↓	$i$	13 $X_c$	14 $X_{ch}$	15 $X_{pr}$	16 $X_{li}$	17 $X_{su}$	18 $X_{aa}$	19 $X_{fa}$	20 $X_{c4}$	21 $X_{pro}$	22 $X_{ac}$	23 $X_{h2}$	24 $X_I$	Rate ( $p_j$ , kg COD·m <sup>-3</sup> ·d <sup>-1</sup> )
1	Disintegration		-1												$f_{xl,xc} k_{dis} X_c$
2	Hydrolysis carbohydrates			$f_{ch,xc}$											$k_{hyd,ch} X_{ch}$
3	Hydrolysis of proteins			-1											$k_{hyd,pr} X_{pr}$
4	Hydrolysis of lipids				-1										$k_{hyd,li} X_{li}$
5	Uptake of sugars						$Y_{su}$								$k_{m,su} \frac{S_{su}}{K_S + S} X_{su} I_1$
6	Uptake of amino acids							$Y_{aa}$							$k_{m,aa} \frac{S_{aa}}{K_S + S_{aa}} X_{aa} I_1$
7	Uptake of LCFA								$Y_{fa}$						$k_{m,fa} \frac{S_{fa}}{K_S + S_{fa}} X_{fa} I_2$
8	Uptake of valerate									$Y_{c4}$					$k_{m,c4} \frac{S_{c4}}{K_S + S_{c4}} X_{c4} \frac{1}{1 + S_{su} / S_{su}}$
9	Uptake of butyrate									$Y_{c4}$					$k_{m,c4} \frac{S_{c4}}{K_S + S_{c4}} X_{c4} \frac{1}{1 + S_{su} / S_{su}}$
10	Uptake of propionate														$k_{m,pr} \frac{S_{pr}}{K_S + S_{pr}} X_{pr} I_2$
11	Uptake of acetate											$Y_{ac}$			$k_{m,ac} \frac{S_{ac}}{K_S + S_{ac}} X_{ac} I_3$
12	Uptake of hydrogen												$Y_{h2}$		$k_{m,h2} \frac{S_{h2}}{K_S + S_{h2}} X_{h2} I_1$
13	Decay of $X_{su}$	1													$k_{dec,su} X_{su}$
14	Decay of $X_{aa}$	1													$k_{dec,aa} X_{aa}$
15	Decay of $X_{fa}$	1							-1						$k_{dec,fa} X_{fa}$
16	Decay of $X_{c4}$	1								-1					$k_{dec,c4} X_{c4}$
17	Decay of $X_{pro}$	1									-1				$k_{dec,pro} X_{pro}$
18	Decay of $X_{ac}$	1										-1			$k_{dec,ac} X_{ac}$
19	Decay of $X_{h2}$	1											-1		$k_{dec,h2} X_{h2}$



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Composites  
(kgCOD·m<sup>-3</sup>)

Carbohydrates  
(kgCOD·m<sup>-3</sup>)

Proteins  
(kgCOD·m<sup>-3</sup>)

Lipids  
(kgCOD·m<sup>-3</sup>)

Sugar degraders  
(kgCOD·m<sup>-3</sup>)

Amino acid degraders  
(kgCOD·m<sup>-3</sup>)

LCFA degraders  
(kgCOD·m<sup>-3</sup>)

Valerate and butyrate  
degraders  
(kgCOD·m<sup>-3</sup>)

Propionate degraders  
(kgCOD·m<sup>-3</sup>)

Acetate degraders  
(kgCOD·m<sup>-3</sup>)

Hydrogen degraders  
(kgCOD·m<sup>-3</sup>)

Particulate inerts  
(kgCOD·m<sup>-3</sup>)

Inhibition factors:  
 $I_1 = \frac{1}{1 + pH/n_{lim}}$   
 $I_2 = \frac{1}{1 + pH/n_{lim} + I_{h2}}$   
 $I_3 = \frac{1}{1 + pH/n_{lim} + NH_3/X_{ac}}$

## Appendix B.1

Kinetic Parameters Used In Aquasim Model, Batstone (1999), Gosset and Belser (1982)

Parameter	Value at 35°C	Unit
$k_{dis}$	0.5	$d^{-1}$
$k_{hyd,CH}$	10	$d^{-1}$
$k_{hyd,PR}$	10	$d^{-1}$
$k_{hyd,LI}$	10	$d^{-1}$
$k_{dec,(X_{aa},X_{su},X_{fa},X_{c4},X_{pro},X_{ac},X_{h2})}$	0.02	$d^{-1}$
$K_{S,NH3,(X_{aa},X_{su},X_{fa},X_{c4},X_{pro},X_{ac},X_{h2})}$	0.0004	$kgCOD/m^3$
$pH_{UL,(acetogenic,acidogenic)}$	5.5	
$pH_{LL,(acetogenic,acidogenic)}$	4	
$k_{m,su}$	30	$kgCOD/kgCOD.d$
$K_{S,su}$	0.5	$kgCOD/m^3$
$Y_{su}$	0.10	$kgCOD/kgCOD$
$k_{m,aa}$	50	$kgCOD/kgCOD.d$
$K_{S,aa}$	0.3	$kgCOD/m^3$
$Y_{aa}$	0.08	$kgCOD/kgCOD$
$k_{m,fa}$	6	$kgCOD/kgCOD.d$
$K_{S,fa}$	0.4	$kgCOD/m^3$
$Y_{fa}$	0.06	$kgCOD/kgCOD$
$K_{LH2,fa}$	$5 \times 10^{-5}$	$kgCOD/m^3$
$k_{m,c4+}$	20	$kgCOD/kgCOD.d$
$K_{S,c4+}$	0.3	$kgCOD/m^3$
$Y_{c4+}$	0.06	$kgCOD/kgCOD$
$K_{LH2,c4+}$	$1 \times 10^{-5}$	$kgCOD/m^3$
$k_{m,pro}$	13	$kgCOD/kgCOD.d$
$K_{S,pro}$	0.3	$kgCOD/m^3$
$Y_{pro}$	0.04	$kgCOD/kgCOD$
$K_{LH2,pro}$	$3.5 \times 10^{-6}$	$kgCOD/m^3$
$k_{m,ac}$	8	$kgCOD/kgCOD.d$
$K_{S,ac}$	0.15	$kgCOD/m^3$
$Y_{ac}$	0.05	$kgCOD/kgCOD$
$pH_{UL,ac}$	7	
$pH_{LL,ac}$	6	
$K_{L,NH3}$	0.0018	$kgCOD/m^3$
$k_{m,h2}$	35	$kgCOD/kgCOD.d$
$K_{S,h2}$	$2.5 \times 10^{-5}$	$kgCOD/m^3$
$Y_{h2}$	0.06	$kgCOD/kgCOD$
$pH_{UL,h2}$	6	
$pH_{LL,h2}$	5	



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