Supplementary material

1. The SWTM model

Nomenclature

C	The concentration (kg COD/m^3)	$k_{s,ac}$	Monod half saturation constant for acetic acid (kg COD·m^{-3})
$C_{CH_4,H}$	The methane concentration which generated from hydrogen (mg/m^3)	$k_{s,alcoho}$	Monod half saturation constant for ethanol (kg COD·m^{-3})
$C_{CH_4,HAC}$	The methane concentration which generated from hydrogen (mg/m^3)	$k_{s,c4}$	Monod half saturation constant for butyric acid (kg COD·m^{-3})
C_{in}	The influent concentration (mg/L)	$k_{s,fa}$	Monod half saturation constant for fatty acid (kg COD·m^{-3})
CO_2	The concentration of carbon dioxide (mg/m^3)	$k_{s,h2}$	Monod half saturation constant for hydrogen (kg COD·m^{-3})
C_{out}	The effluent concentration (mg/L)	$k_{s,homo}$	Monod half saturation constant for homoacetogenesis (kg COD·m^{-3})
$f_{alcohol}$	Yield of ethanol on sugar (kg COD·kg COD^{-1})	$k_{s,lac}$	Monod half saturation constant for lactic acid (kg COD·m^{-3})
dC	The concentration variation (mg/L)	$k_{s,pr}$	Monod half saturation constant for proteins (kg COD·m^{-3})
f_{lactic}	Yield of lactic acid on sugar (kg COD (lactic acid)·kg COD^{-1} (sugar))	$k_{s,su}$	Monod half saturation constant for sugar (kg COD·m^{-3})
$f_{ac,aa}$	Yield of acetic acid on amino acid (kg COD (acetic acid)·kg COD^{-1} (amino acid))	$k_{SO4,ac}$	Half saturation coefficient for the uptake of sulfate with acetic acid (kmol/m^3)
$f_{ac,fa}$	Yield of acetic acid on fatty acid (kg COD (acetic acid)·kg COD^{-1} (fatty acid))	$k_{SO_4,i}$	Half saturation coefficient of component i on sulfate reduction process

			(kmol/m^3)
$f_{ac,lac}$	Yield of acetic acid on lactic acid (kg COD (acetic acid)·kg COD^{-1} (lactic acid))	$k_{SO4,bu}$	Half saturation coefficient for the uptake of sulfate with butyric acid (kmol/m^3)
$f_{ac,su}$	Yield of acetic acid on sugar (kg COD (acetic acid)·kg COD^{-1} (sugar))	$k_{SO4,pro}$	Half saturation coefficient for the uptake of sulfate with propoinic acid (kmol/m^3)
$f_{alcohol,su}$	Yield of ethanol on sugar (kg COD (ethanol)·kg COD^{-1} (sugar))	NH_3	The ammonia concentration (mg/L)
$f_{bu,aa}$	Yield of butyric acid on amino acid (kg COD (butyric acid)·kg COD^{-1}(amino acid))	r_i^f	Concentration generation (consumption) rate in the model (mg/L/min)
$f_{bu,su}$	Yield of butyric acid on sugar (kg COD (butyric acid)·kg COD^{-1}(sugar))	S^{2-}	The concentration of sulfion (kg COD/m^3)
$f_{ch,xc}$	yield of lipids on NBCOD (kg COD (lipids)·kg COD^{-1} (NBCOD))	S_{aa}	The concentration of amino acid (kg COD/m^3)
$f_{fa,li}$	yield of fatty on lipids (kg COD (fatty acid)·kg COD^{-1} (lipids))	S_{ac}	The concentration of acetic acid (kg COD/m^3)
$f_{h2,aa}$	Yield of hydrogen on amino acid (kg H_2·kg COD^{-1})	$S_{alcohol}$	The concentration of ethanol (kg COD/m^3)
$f_{h2,fa}$	Yield of hydrogen on fatty acid (kg H_2·kg COD^{-1})	S_{bu}	The concentration of butyric acid (kg COD/m^3)
$f_{h2,su}$	Yield of hydrogen on sugar (kg H_2·kg COD^{-1})	S_{ch4}	The concentration of methane (mg/m^3)
$f_{lac,su}$	Yield of lactic acid on sugar (kg COD (lactic acid)·kg COD^{-1} (sugar))	S_{fa}	The concentration of fatty acid (kg COD/m^3)
$f_{li,xc}$	yield of lipids on NBCOD (kg COD (lipids)·kg COD^{-1}(NBCOD))	S_{for}	The concentration of formic acid (kg COD/m^3)

$f_{pr,xc}$	yield of proteins on NBCOD (kg COD (protein)·kg COD^{-1} (NBCOD))	S_{h2}	The concentration of hydrogen (mg/m^3)
$f_{pro,aa}$	Yield of propionic acid on amino acid (kg COD (propionic acid)·kg COD^{-1} (amino acid))	S_i	Carbon content of the component i (kg COD/m^3)
$f_{pro,lac}$	Yield of propoinic acid on lactic acid (kg COD (propionic acid)·kg COD^{-1} (lactic acid))	S_{lactic}	The concentration of lactic acid (kg COD/m^3)
$f_{pro,su}$	Yield of propionic acid on sugar (kg COD (propionic acid)·kg COD^{-1} (sugar))	S_{NO_X}	The concentration of nitrate or nitrite (kg COD/m^3)
f_{urea}	Yied of urea (kg COD·kg COD^{-1})	S_{SO_4}	The concentration of sulfate (kg COD/m^3)
i	component index (see supplementary material)	SO_4^{2-}	The concentration of sulfate (kg COD/m^3)
j	process index (see supplementary material)	S_{pro}	The concentration of propionic acid (kg COD/m^3)
k_{ac}	Half saturation coefficient of acetic acid on sulfate reduction process (kg COD/m^3)	*SRB*	The amount of SRB (Copies/mL)
$k_{alcohol}$	Half saturation coefficient of ethanol (kmol/m^3)	S_{su}	The concentration of sugar (kg COD/m^3)
k_{bu}	Half saturation coefficient of butyric acid on sulfate reduction process (kg COD/m^3)	S_{va}	The concentration of valeric acid (kg COD/m^3)
$k_{dec,aa}$	first order decay rate for X_{aa} death (d^{-1})	t	Time (d)
$\mathrm{k}_{\mathrm{dec},\mathrm{X}_{\mathrm{ac}}}$	first order decay rate for X_{ac} death (d^{-1})	*Urea*	The concentration of urea (kg urea/m^3)
$\mathrm{k}_{\mathrm{dec},\mathrm{X}_{\mathrm{alcohol}}}$	first order decay rate for $X_{alcohol}$ death (d^{-1})	X	The concentration of particulate component (kg COD/ m^3)

$k_{dec,X_{bu}}$	first order decay rate for X_{bu} death (d^{-1})	X_{aa}	The amount of acetic ammonify bacteria (Copies/mL)
$k_{dec,X_{h2}}$	first order decay rate for X_{h2} death (d^{-1})	X_{ac}	The amount of acetic acid uptake microorganism (Copies/mL)
$k_{dec,X_{homo}}$	first order decay rate for X_{homo} death (d^{-1})	X_{alcoho}	The amount of ethanol uptake microorganism (Copies/mL)
$k_{dec,X_{lactic}}$	first order decay rate for X_{lactic} death (d^{-1})	X_{bu}	The amount of butyric acid uptake microorganism (Copies/mL)
$k_{dec,X_{pro}}$	first order decay rate for X_{pro} death (d^{-1})	X_c	The concentration of NBCOD (kg COD/m^3)
$k_{dec,XSRB}$	first order decay rate for SRB death (d^{-1})	X_{ch}	The concentration of polysaccharide (kg COD/m^3)
$k_{hyd,xc}$	Hydrolysis rate constant for NBCOD (d^{-1})	X_{h2}	Homoacetogenic bacteria (Copies/mL)
$k_{H2S,ac}$	Monod maximum specific uptake rate of acetic acid to H_2S (kg COD /kg COD ·d^{-1})	X_{homo}	The amount of homoacetogenic bacteria (Copies/mL)
$k_{H2S,bu}$	Monod maximum specific uptake rate of butyric acid to H_2S (kg COD /kg COD ·d^{-1})	x_{lactic}	The amount of lactic acid uptake microorganism (Copies/mL)
$k_{H2S,pro}$	Monod maximum specific uptake rate of propionic acid to H_2S (kg COD /kg COD ·d^{-1})	X_{li}	The concentration of lipids (kg COD/m^3)
$k_{H_2S,i}$	Monod maximum specific uptake rate for sulfate reduction process with carbon source *i* (kg COD /kg COD ·d^{-1})	X_{pr}	The concentration of proteins (kg COD/m^3)
k_{hyd}	Hydrolysis rate constant (d^{-1})	X_{pro}	The amount of propionic acid uptake microorganism (Copies/mL)
$k_{hyd,ch}$	Hydrolysis rate constant for	X_{SRB}	The amount of SRB (Copies/mL)

	polysaccharide (d^{-1})		
$k_{hyd,li}$	Hydrolysis rate constant for lipids (d^{-1})	Y_{aa}	yield of biomass on amino acid (kg COD-biomass /kg COD-substrate)
$k_{hyd,pr}$	Hydrolysis rate constant for proteins (d^{-1})	Y_{ac}	yield of biomass on acetic acid (kg COD-biomass /kg COD-substrate)
$k_{hyd,urea}$	Hydrolysis rate constant for urea (d^{-1})	$Y_{alcohol}$	yield of biomass on ethanol (kg COD-biomass /kg COD-substrate)
k_{lactic}	Half saturation coefficient of lactic acid (kg COD/m^3)	Y_{c4}	yield of biomass on butyric acid (kg COD -biomass/kg COD-substrate)
$k_{m,aa}$	specific Monod maximum uptake rate of amino acid (kg COD-substrate /kg COD -biomass·d^{-1})	Y_{fa}	yield of biomass on fatty acid (kg COD-biomass /kg COD-substrate)
$k_{m,ac}$	specific Monod maximum uptake rate of acetic acid (kg COD-substrate /kg COD-biomass ·d^{-1})	Y_{h2}	yield of biomass on hydrogen (kg COD-biomass /kg COD-substrate)
$k_{m,alcohol}$	specific Monod maximum uptake rate of ethanol (kg COD-substrate /kg COD-biomass ·d^{-1})	Y_{homo}	yield of biomass on homoacetogenesis process (kg COD-biomass /kg COD-substrate)
$k_{m,c4}$	specific Monod maximum uptake rate of butyric acid (kg COD-substrate /kg COD-biomass ·d^{-1})	Y_{lac}	yield of biomass on lactic acid (kg COD-biomass /kg COD-substrate)
$k_{m,fa}$	specific Monod maximum uptake rate of fatty acid (kg COD-substrate /kg COD-biomass ·d^{-1})	Y_{pro}	yield of biomass on propionic acid (kg COD-biomass /kg COD-substrate)
$k_{m,h2}$	specific Monod maximum uptake rate of hydrogen (kg COD-substrate /kg COD-biomass ·d^{-1})	Y_{SRB}	Yield of SRB (kg COD-biomass /kg COD-substrate)
$k_{m,homo}$	specific Monod maximum uptake rate in homoacetogenesis process	Y_{su}	yield of biomass on sugar (kg COD-biofilm /kg COD-substrate)

	(kg COD-substrate /kg COD-biomass ·d^{-1})		
$k_{m,lactic}$	specific Monod maximum uptake rate of lactic acid (kg COD-substrate /kg COD-biomass ·d^{-1})	$y_{m,i}$	The measurement result
$k_{m,pr}$	specific Monod maximum uptake rate of propionic acid (kg COD-substrate /kg COD-biomass ·d^{-1})	y_i	The simulation result
$k_{m,su}$	specific Monod maximum uptake rate of sugar (kg COD-substrate /kg COD-biomass ·d^{-1})	$\bar{y}$	The average value of the measurement results
$k_{NO_x,i}$	Carbon source utilization rate constant by N-oxide degrade with carbon source *i* (day^{-1})	*Greek letter*	
k_{pro}	Half saturation coefficient of propionic acid on sulfate reduction process (kg COD/m^3)	ρ_j^f	Kinetic rate equation of process *j* (see supplementary material)
$k_{s,aa}$	Monod half saturation constant for amino acid (kg COD·m^{-3})	$v_{j,i}$	rate coefficients for component *i* on process *j*

Similar to Active sludge model, the model was summarized in Table S1 and Table S2. Table S1 consists of the biochemical rate coefficients for organic matters (v_{ij}) and Table S2 consists of each kinetic rate equations (ρ_j). The processes index in Table S1 corresponds to that in Table S2.

Table S1 Biochemical rate coefficients ($\nu_{i,j}$) for organic components in sewer

Components	S_{aa}	S_{su}	S_{fa}	S_{bu}	S_{pro}	S_{lactic}	S_{ac}	$S_{alcohol}$	S_{ch4}	S_{h2}	NH_3	X_{bu}	X_{pro}	X_{ac}	X_{lactic}	X_{alcoho}	X_{homo}	X_{h2}	X_{aa}
1		-1		$(1-Y_{su})*f_{bu,su}$	$(1-Y_{su})*f_{pro,su}$	$(1-Y_{su})*f_{lac,su}$	$(1-Y_{su})*f_{ac,su}$	$(1-Y_{su})*f_{alcohol,su}$		$(1-Y_{su})*f_{h2,su}$									
2	-1			$(1-Y_{aa})*f_{bu,aa}$	$(1-Y_{aa})*f_{pro,aa}$		$(1-Y_{aa})*f_{ac,aa}$			$(1-Y_{aa})*f_{h2,aa}$	$(1-Y_{aa})*f_{nh3,aa}$								Y_{aa}
3.			-1				$(1-Y_{fa})*f_{ac,fa}$			$(1-Y_{fa})*f_{h2,fa}$									
4.				-1			$0.8*(1-Y_{C4})$			$0.2*(1-Y_{C4})$		Y_{c4}							
5.					-1		$0.57*(1-Y_{pro})$			$0.43*(1-Y_{pro})$			Y_{pro}						
6.					$(1-Y_{lac})*f_{pro,lac}$	-1	$(1-Y_{lac})*f_{ac,lac}$								Y_{latic}				
7.							$0.8*(1-Y_{alkhol})$	-1		$0.2*(1-Y_{alkhol})$						$Y_{alcohol}$			
8.							$1-Y_{homo}$			-1									
9.							-1		$(1-Y_{ac})$					Y_{ac}					
10.									$(1-Y_{h2})$	-1								Y_{h2}	
11.												-1							
12.													-1						
13.														-1					
14.																		-1	
15.																-1			
16.															-1				
17.																	-1		

Note: The blank in table represents zero.

Continued from Table S1

Components	S_{va}	S_{for}	S_{bu}	S_{pro}	S_{ac}	S_{h2}	Saa	Urea	NH_3	CO_2	SO_4^{2-}	S^{2-}	X_{aa}	SRB
Ammonification														
18.								-1	f_{urea}	1-f_{urea}				
19													-1	
Sulfate reduction														
20			-1		(1-Y_{srb})*0.7						(Y_{srb}-1)*0.3/64	(1-Y_{srb})*0.3/64		Y_{srb}
21				-1	(1-Y_{srb})*0.57						(Y_{srb}-1)*0.43/64	(1-Y_{srb})*0.43/64		
22					-1						(Y_{srb}-1)/64	(1-Y_{srb})/64		
23														-1

Hydrolyzation

Components	X_C	X_{ch}	X_{pr}	S_{aa}	S_{aa}	S_{fa}	S_{su}	X_{li}
24	-1	$f_{ch,xc}$	$f_{pr,xc}$					$f_{li,xc}$
25			-1	1				
26					1-$f_{fa,li}$	$f_{fa,li}$		-1
27		-1					1	

Table S2 Kinetic rate equations (ρ_j) for organic matters in sewer

Processes	Equation	References
1. Uptake of sugars	$k_{m,su}\frac{S_{su}}{k_{s,su}+S_{su}}X_{su}$	(vavilin., 2002)
2. Uptake of amino acid	$k_{m,aa}\frac{S_{aa}}{k_{s,aa}+S_{aa}}X_{aa}$	(vavilin., 2002)
3.Uptake of LAFC	$k_{m,fa}\frac{S_{fa}}{k_{s,fa}+S_{fa}}X_{fa}$	(vavilin., 2002)
4.Uptake of butyric acid	$k_{m,c4}\frac{S_{bu}}{k_{s,bu}+S_{bu}}X_{bu}$	(vavilin., 2002)
5.Uptake of propionic acid	$k_{m,pr}\frac{S_{pro}}{k_{s,pro}+S_{pro}}X_{pro}$	(vavilin., 2002)
6.Uptake of lactic acid	$k_{m,lactic}\frac{S_{latic}}{k_{s,lac}+S_{latic}}X_{lactic}$	(Hinken et al., 2014)
7.Uptake of ethanol	$k_{m,alcoho}\frac{S_{alcoho}}{k_{s,alcoho}+S_{alcoho}}X_{alcoho}$	(Chen et al., 2009)
8. Homoacetogenesis process	$k_{m,homo}\frac{S_{h2}}{k_{s,homo}+S_{h2}}X_{homo}$	(Tugtas et al., 2010)
9.Uptake of acetic acid	$k_{m,ac}\frac{S_{ac}}{k_{s,ac}+S_{ac}}X_{ac}$	(vavilin., 2002)
10.Uptake of hydrogen	$k_{m,h2}\frac{S_{h2}}{k_{s,h2}+S_{h2}}X_{h2}$	(vavilin., 2002)
11.Decay of X_{bu}	$k_{dec,X_{bu}}X_{bu}$	(vavilin., 2002)
12.Decay of X_{pro}	$k_{dec,X_{pro}}X_{pro}$	(vavilin., 2002)
13.Decay of X_{ac}	$k_{dec,X_{ac}}.X_{ac}$	(vavilin., 2002)
14.Decay of X_{h2}	$k_{dec,X_{h2}}X_{h2}$	(vavilin., 2002)
15.Decay of $X_{alcohol}$	$k_{dec,X_{alcoho}}X_{alcoho}$	(Chen et al., 2009)
16.Decay of X_{lactic}	$k_{dec,X_{latic}}X_{latic}$	(Hinken et al., 2014)
17.Decay of X_{homo}	$k_{dec,X_{homo}}X_{homo}$	(Antonopoulou et al., 2012)
18.Hydrolysis of urea	$k_{hyd,urea}$*urea	
19. .Decay of X_{aa}	$k_{dec,aa}$*X_{aa}	(vavilin., 2002)
20.Sulfate reduction with butyric acid	$k_{H2S,bu}\frac{S_{bu}}{k_{bu}+S_{bu}}\cdot\frac{S_{SO4}}{k_{SO4,bu}+S_{SO4}}\cdot X_{SRB}$	(Barrera et al., 2015)
21.Sulfate reduction with propionic acid	$k_{H2S,pro}\frac{S_{pro}}{k_{pro}+S_{pro}}\cdot\frac{S_{SO4}}{k_{SO4,pro}+S_{SO4}}\cdot X_{SRB}$	(Barrera et al., 2015)
22. Sulfate reduction with acetic acid	$k_{H2S,ac}\frac{S_{ac}}{k_{ac}+S_{ac}}\cdot\frac{S_{SO4}}{k_{SO4,ac}+S_{SO4}}\cdot X_{SRB}$	(Barrera et al., 2015)
23.Decay of SRB	$k_{dec,X_{SRB}}X_{SRB}$	(vavilin., 2002)
24. Hydrolysis of NBCOD	$k_{hyd,\ Xc}X_C$	(vavilin., 2002)
25 Hydrolysis of proteins	$k_{hyd,\ pr}X_{pr}$	(vavilin., 2002)

26.Hydrolysis of lipids	$k_{hyd,li}X_{li}$	(vavilin., 2002)
27. Hydrolysis of polysaccharide	$k_{hyd,ch}X_{ch}$	(vavilin., 2002)

Table S3 Kinetic parameter values used in the model.

Symbol	Units	Value	References
$f_{ac,aa}$	kg COD (acetic acid)·kg COD^{-1}(amino acid)	0.4	(vavilin., 2002)
$f_{ac,fa}$	kg COD(acetic acid)·kg COD^{-1}(fatty acid)	0.31	(vavilin., 2002)
$f_{ac,lac}$	kg COD (acetic acid)·kg COD^{-1}(lactic acid)	0.222	(Antonopoulou et al., 2012)
$f_{ac,su}$	kg COD (acetic acid)·kg COD^{-1} (sugar)	0.041	calibrated
$f_{alcohol,su}$	kg COD (ethanol)·kg COD^{-1} (sugar)	0.09	calibrated
$f_{bu,aa}$	kg COD (butyric acid)·kg COD^{-1} (amino acid)	0.26	(vavilin., 2002)
$f_{bu,su}$	kg COD (butyric acid)·kg COD^{-1} (sugar)	0.078	calibrated
$f_{ch,xc}$	kg COD·kg COD^{-1}	0.2	(vavilin., 2002)
$f_{fa.li}$	kg COD (fatty acid)·kg COD^{-1} (lipids)	0.95	(vavilin., 2002)
$f_{h2,aa}$	kg COD (H_2)·kg COD^{-1} (amino acid)	0.06	(vavilin., 2002)
$f_{h2,fa}$	kg COD (H_2)·kg COD^{-1} (fatty acid)	0.26	(vavilin., 2002)
$f_{h2,su}$	kg COD (H_2)·kg COD^{-1} (sugar)	0.19	(vavilin., 2002)
$f_{lac,su}$	kg COD (lactic acid)·kg COD^{-1} (sugar)	0.000028	calibrated
$f_{li,xc}$	kg COD (lipids) ·kg COD^{-1} (NBCOD)	0.25	(vavilin., 2002)
$f_{nh3,aa}$	kg N/kg COD	0.186	calibrated
$f_{pr,xc}$	kg COD (protein)·kg COD^{-1} (NBCOD)	2000	(vavilin., 2002)
$f_{pro,aa}$	kg COD (propionic acid)·kg COD^{-1} (amino acid)	0.05	(vavilin., 2002)
$f_{pro,lac}$	kg COD (propionic acid) ·kg COD^{-1} (lactic acid)	7.78	calibrated
$f_{pro,su}$	kg COD (propionic acid) ·kg COD^{-1} (sugar)	0.13	(vavilin., 2002)
f_{urea}	kg N·kg COD^{-1}	0.466	calibrated
k_{ac}	kg COD/m^3	0.05	(Barrera et al., 2015)
k_{bu}	kg COD/m^3	0.015	(Barrera et al., 2015)
$k_{dec,aa}$	d^{-1}	0.020	calibrated

$k_{dec,X_{ac}}$	d^{-1}	0.020	calibrated
$k_{dec,X_{alcohol}}$	d^{-1}	0.8	calibrated
$k_{dec,X_{bu}}$	d^{-1}	0.03	(vavilin., 2002)
$k_{dec,xfa}$	d^{-1}	0.02	calibrated
$k_{dec,X_{h2}}$	d^{-1}	0.009	calibrated
$k_{dec,X_{homo}}$	d^{-1}	0.03	(Antonopoulou et al., 2012)
$k_{dec,X_{lactic}}$	d^{-1}	0.01	calibrated
$k_{dec,X_{pro}}$	d^{-1}	0.01	(vavilin., 2002)
$k_{dec,XSRB}$	d^{-1}	0.02	(Barrera et al., 2015)
$k_{H2S,ac}$	kg COD-sulfate/kg COD-carbon source ·d^{-1}	0.0063	(Barrera et al., 2015)
$k_{H2S,bu}$	kg COD-sulfate/kg COD-carbon source ·d^{-1}	0.0070	(Barrera et al., 2015)
$k_{H2S,pro}$	kg COD-sulfate/kg COD-carbon source ·d^{-1}	0.0075	(Barrera et al., 2015)
$k_{hyd,ch}$	d^{-1}	106	calibrated
$k_{hyd,li}$	d^{-1}	0.17	calibrated
$k_{hyd,pr}$	d^{-1}	0.02	calibrated
$k_{hyd,urea}$	d^{-1}	1.566	calibrated
$k_{m,aa}$	kg COD-substrate/kg COD-biomass ·d^{-1}	53	calibrated
$k_{m,ac}$	kg COD-substrate/kg COD-biomass ·d^{-1}	32	calibrated
$k_{m,alcohol}$	kg COD-substrate/kg COD-biomass ·d^{-1}	0.1	calibrated
$k_{m,c4}$	kg COD-substrate/kg COD-biomass ·d^{-1}	22	(vavilin., 2002)
$k_{m,fa}$	kg COD-substrate/kg COD-biomass ·d^{-1}	11	calibrated
$k_{m,h2}$	kg COD-substrate/kg COD-biomass ·d^{-1}	25	calibrated
$k_{m,homo}$	kg COD-substrate/kg COD-biomass ·d^{-1}	28.5	(Antonopoulou et al., 2012)
$k_{m,lactic}$	kg COD-substrate/kg COD-biomass ·d^{-1}	45	(vavilin., 2002)
$k_{m,pr}$	kg COD-substrate/kg COD-biomass ·d^{-1}	21	calibrated
$k_{m,su}$	kg COD-substrate/kg COD-biomass ·d^{-1}	26	calibrated
k_{pro}	kg COD/m^3	0.02	(Barrera et al., 2015)

$k_{s,aa}$	kg COD/m^3	1.198	calibrated
$k_{s,ac}$	kg COD/m^3	0.035	(vavilin., 2002)
$k_{s,alcoho}$	kg COD/m^3	0.8	calibrated
$k_{s,c4}$	kg COD/m^3	0.062	calibrated
$k_{s,bu}$	kg COD/m^3	0.080	calibrated
$k_{s,fa}$	kg COD/m^3	1	(vavilin., 2002)
$k_{s,h2}$	kg COD/m^3	0.0006	calibrated
$k_{s,homo}$	kg COD/m^3	0.7*10^{-6}	(Antonopoulou et al., 2012)
$k_{s,lac}$	kg COD/m^3	0.5	(Antonopoulou et al., 2012)
$k_{s,pro}$	kg COD/m^3	0.021	calibrated
$k_{s,su}$	kg COD/m^3	0.022	calibrated
$k_{SO4,ac}$	kmol/m^3	0.0001	(Barrera et al., 2015)
$k_{SO4,bu}$	kmol/m^3	0.002	(Barrera et al., 2015)
$k_{SO4,pro}$	kmol/m^3	0.0023	(Barrera et al., 2015)
Y_{aa}	kg COD-biomass/kg COD-substrate	0.08	(vavilin., 2002)
Y_{ac}	kg COD-biomass/kg COD-substrate	0.05	(vavilin., 2002)
Y_{alohol}	kg COD-biomass/kg COD-substrate	0.9	calibrated
Y_{c4}	kg COD-biomass/kg COD-substrate	0.04	(vavilin., 2002)
Y_{fa}	kg COD-biomass/kg COD-substrate	0.06	(vavilin., 2002)
Y_{h2}	kg COD-biomass/kg COD-substrate	0.06	(vavilin., 2002)
Y_{homo}	kg COD-biomass/kg COD-substrate ·d^{-1}	0.06	(Antonopoulou et al., 2012)
Y_{lac}	kg COD-biomass·kg COD^{-1}-substrate	0.9	calibrated
Y_{pro}	kg COD-biomass/kg COD-substrate	0.04	(vavilin., 2002)
Y_{su}	kg COD-biomass/kg COD-substrate	0.1	(vavilin., 2002)

Table S4 Goodness of fit statistics in the study

Figure	Data series	R^2	Figure	Data series	R^2
Fig. 3	TB simulation	0.9820	Fig. 4 (b)	Hydrogen simulation	0.9804
Fig. 3	SRB simulation	0.9806	Fig. 5 (a)	Protein simulation	0.9903
Fig. 3	HPA simulation	0.9817	Fig. 5 (a)	Ammonia simulation	0.9914
Fig. 3	AB simulation	0.9518	Fig. 5 (a)	Urea simulation	0.9991
Fig. 3	MA simulation	0.9883	Fig. 5 (a)	Amino acid simulation	0.9889
Fig. 4 (a)	Butyric acid simulation	0.9910	Fig. 5 (a)	TN simulation	0.9994
Fig. 4 (a)	Propionic acid simulation	0.9887	Fig. 5 (a)	Ammonia simulation	0.9771
Fig. 4 (a)	Acetic acid simulation	0.9923	Fig. 5 (a)	Protein simulation	0.9824
Fig. 4 (a)	VFA simulation	0.9855	Fig. 5 (a)	Urea simulation	0.9893
Fig. 4 (a)	Lactic acid simulation	0.9894	Fig. 5 (b)	Sulfate simulation	0.9631
Fig. 4 (a)	Alcohol simulation	0.9921	Fig. 5 (b)	Hydrogen sulfate simulation	0.9124
Fig. 4 (b)	Methane simulation	0.9781	Fig. 6 (b)	Sulfate reduction Propionic acid measurement	0.9805
Fig. 4 (b)	CO_2 simulation	0.9701	Fig. 6 (b)	Acetic acid simulation	0.9901
Fig. 4 (b)	H_2S simulation	0.9866	Fig. 6 (b)	Butyric acid simulation	0.9906

2 Pollutants analysis

The measurement methods for VFA, ethanol, lactic acid and other pollutants are described as follows. Except before the analysis of protein lipids and carbohydrates, water samples were filtered by a 0.45μm membrane before the pollutant measurements.

2.1 VFA

VFA was measured by gas chromatography (GC-2014 Shimadzu, Japan) equipped with a flame ionization detector and a PE WAX ETR column. The oven was first held at 100°C for 2 min and then heated to 160°C with a heating rate of 3 °C/min. The carrier gas consisted of N_2, H_2 and air, and the corresponding flow rate were 20 mL/min, 35 mL/min and 350 mL/min, respectively.

2.2 Ethanol

Ethanol was also measured by gas chromatography (GC-2014 Shimadzu, Japan) with flame ionization. Oven was maintained at 40°C for 5 min, before it was increased at a rate of 10 °C/min to 90°C for 5 min. Temperature was then further increased by 10 °C/min to 150°C and head for 2 min. After this protocol was implemented, 1 μL of the sample was injected. The carrier gas consisted of N_2, H_2 and air, and the corresponding flow rates were 35.3 mL/min, 35 mL/min and 350 mL/min, respectively.

2.3 Lactic acid

High-performance liquid chromatography (HPLC, LC-2010AHT) from Shimadzu Corporation equipped with a UV detector (λ = 205 nm) and a hypersil BDS C18 column was used to measure the concentration of lactic acid (Jin et al., 2015). The mobile phase consisted of methanol and water (10:90) (V/V). The flow rate was maintained at 0.7 mL/min, and the column temperature was 35°C.

2.4 Amino acids

Amino acid analysis was carried out after precolumn derivatization with phenylisothiocyanate (PITC) (Heinrikson and Meridith, 1984). First, 300 μL 1 mol/L coupling buffer (a solvent mixture with acetonitrile and triethylamine) and 100 μL 0.1 mol/L solvent mixture with PITC and acetonitrile were added into each sample (500 μL). After samples stood for 1 hour under darkness, 800 μL n-hexane was added into each sample. Finally, via centrifugation (1000 r and 5 min), the lower liquid was extracted for the further measurement.

The extracted solution were measured by HPLC (LC-2010AHT). The mobile phase contained a gradient-programmed mixture of solvent A (0.05 M sodium acetate) and solvent B (0.1 M sodium acetate in 40% acetonitrile and 10% methanol).

2.5 Carbohydrates and glucose

Carbohydrates were determined by the anthrone method at 620 nm (Loewus, 1952). In addition, glucose was measured by HPLC (LC-2010AHT) with a Supelco Kromasil NH_2 column (Rahman, 2008). The mobile phase consisted of acetonitrile and water (80:20) (V/V). The oven was set 30 °C, and the flow rate was set to 0.6 mL/min.

2.6 Other pollutants

CH_4, H_2 and H_2S were measured by gas chromatography (GC-2014 Shimadzu, Japan) (Jin et al., 2015). CO_2 was measured by a JSA5-CO_2-IR gas analyzer (JSA5-CO_2-IR, Shenzhen Jishunan Technology Co., China) equipped with an infrared sensor. The national standard methods were used to measure the concentrations of COD, NH_3-N, NO_3-N, ammonia, total nitrogen and sulfate (Jin et al., 2015). Values of DO, pH and ORP were analyzed using an HQ30d acidometer (HACH, USA) (Yu et al., 2009). Urea was directly determined by the p-dimethylaminobenzaldehyde method. Protein was monitored using the folin-phenol reagent method (Lowry et al., 1951). Lipids were analyzed by the gravimetric method according to the previous study (Woertz et ai., 2009).

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