Supplementary Table II. Kinetic rate expressions for microbial reactions

Process	**Rate equations [g m^{-3} day^{-1}]**
Autotrophic (AOB)	
1. Aerobic growth	$\mu_{\mathrm{AOB}} \cdot \frac{S_{\mathrm{NH4}}}{S_{\mathrm{NH4}} + K_{\mathrm{NH4}}^{\mathrm{AOB}}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{AOB}}} \cdot X_{\mathrm{AOB}}$
2. Lysis	$b_{\mathrm{AOB}} \cdot X_{\mathrm{AOB}}$
Autotrophic (NOB)	
3. Aerobic growth	$\mu_{\mathrm{NOB}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{NOB}}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{NOB}}} \cdot X_{\mathrm{NOB}}$
4. Lysis	$b_{\mathrm{NOB}} \cdot X_{\mathrm{NOB}}$
Heterotrophic (Het)	
5. Aerobic growth on S_{F}	$\mu_{\mathrm{Het}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + K_{\mathrm{S\_F}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{A}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
6. Aerobic growth on S_{A}	$\mu_{\mathrm{Het}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + K_{\mathrm{S\_A}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
7. Anoxic (NO_2) growth on S_{F}	$\mu_{\mathrm{Het}} \cdot \eta_{\mathrm{Het}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + K_{\mathrm{S\_F}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{Het}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
8. Anoxic (NO_2) growth on S_{A}	$\mu_{\mathrm{Het}} \cdot \eta_{\mathrm{Het}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + K_{\mathrm{S\_A}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{Het}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
9. Anoxic (NO_3) growth on S_{F}	$\mu_{\mathrm{Het}} \cdot \eta_{\mathrm{Het}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + K_{\mathrm{S\_F}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{F}}}{S_{\mathrm{F}} + S_{\mathrm{A}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{Het}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
10. Anoxic (NO_3) growth on S_{A}	$\mu_{\mathrm{Het}} \cdot \eta_{\mathrm{Het}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + K_{\mathrm{S\_A}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + S_{\mathrm{F}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{Het}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot X_{\mathrm{Het}}$
11. Fermentation	$q_{\mathrm{fe}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{Het}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{Het}}} \cdot \frac{K_{\mathrm{NO3}}^{\mathrm{Het}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{Het}}} \cdot \frac{S_{\mathrm{f}}}{S_{\mathrm{f}} + K_{\mathrm{fe}}} \cdot X_{\mathrm{Het}}$
12. Lysis	$b_{\mathrm{Het}} \cdot X_{\mathrm{Het}}$
PAO	
13. Anaerobic storage of PHA	$q_{\mathrm{PHA}}^{\mathrm{PAO}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + K_{\mathrm{S\_A}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PP}} / X_{\mathrm{PAO}}}{X_{\mathrm{PP}} / X_{\mathrm{PAO}} + K_{\mathrm{PP}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}} + K_{\mathrm{GLY}}^{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
14. Aerobic storage of PP	$q_{\mathrm{PP}}^{\mathrm{PAO}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{S_{\mathrm{PO4}}}{S_{\mathrm{PO4}} + K_{\mathrm{PO4}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA\_PP}}^{\mathrm{PAO}}} \cdot \frac{K_{\mathrm{MP}}^{\mathrm{PAO}} - X_{\mathrm{PP}} / X_{\mathrm{PAO}}}{K_{\mathrm{IP}}^{\mathrm{PAO}} + (K_{\mathrm{MP}}^{\mathrm{PAO}} - X_{\mathrm{PP}} / X_{\mathrm{PAO}})} \cdot X_{\mathrm{PAO}}$
15. Aerobic growth	$\mu_{\mathrm{PAO}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA}}^{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
16. Aerobic storage of GLY	$q_{\mathrm{GLY}}^{\mathrm{PAO}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA\_GLY}}^{\mathrm{PAO}}} \cdot \frac{K_{\mathrm{MG}}^{\mathrm{PAO}} - X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}}}{K_{\mathrm{IG}}^{\mathrm{PAO}} + (K_{\mathrm{MG}}^{\mathrm{PAO}} - X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}})} \cdot X_{\mathrm{PAO}}$
17. Anoxic (NO2) storage of PP	$q_{\mathrm{PP}}^{\mathrm{PAO}} \cdot \eta_{\mathrm{PAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{PAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{PAO}}} \cdot \frac{S_{\mathrm{PO4}}}{S_{\mathrm{PO4}} + K_{\mathrm{PO4}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA\_PP}}^{\mathrm{PAO}}} \cdot \frac{K_{\mathrm{MP}}^{\mathrm{PAO}} - X_{\mathrm{PP}} / X_{\mathrm{PAO}}}{K_{\mathrm{IP}}^{\mathrm{PAO}} + (K_{\mathrm{MP}}^{\mathrm{PAO}} - X_{\mathrm{PP}} / X_{\mathrm{PAO}})} \cdot X_{\mathrm{PAO}}$
18. Anoxic (NO_2) growth	$\mu_{\mathrm{PAO}} \cdot \eta_{\mathrm{PAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{PAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA}}^{\mathrm{PAO}}} \cdot X_{\mathrm{PAO}}$
19. Anoxic (NO_2) storage of GLY	$q_{\mathrm{GLY}}^{\mathrm{PAO}} \cdot \eta_{\mathrm{PAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{PAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{PAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{PAO}}} \cdot \frac{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}}}{X_{\mathrm{PHA,P}} / X_{\mathrm{PAO}} + K_{\mathrm{PHA\_GLY}}^{\mathrm{PAO}}} \cdot \frac{K_{\mathrm{MG}}^{\mathrm{PAO}} - X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}}}{K_{\mathrm{IG}}^{\mathrm{PAO}} + (K_{\mathrm{MG}}^{\mathrm{PAO}} - X_{\mathrm{GLY,P}} / X_{\mathrm{PAO}})} \cdot X_{\mathrm{PAO}}$
20. Lysis of PAO	$b_{\mathrm{PAO}} \cdot X_{\mathrm{PAO}}$
21. Lysis of PP	$b_{\mathrm{PP}} \cdot X_{\mathrm{PP}}$
22. Lysis of PHA	$b_{\mathrm{PHA}} \cdot X_{\mathrm{PHA,P}}$

23. Lysis of GLY	$b_{\mathrm{GLY}} \cdot X_{\mathrm{GLY,P}}$

GAO

24. Anaerobic storage of PHA	$q_{\mathrm{PHA}}^{\mathrm{GAO}} \cdot \frac{S_{\mathrm{A}}}{S_{\mathrm{A}} + K_{\mathrm{S\_A}}^{\mathrm{GAO}}} \cdot \frac{X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}} + K_{\mathrm{GLY}}^{\mathrm{GAO}}} \cdot X_{\mathrm{GAO}}$
25. Aerobic growth	$\mu_{\mathrm{GAO}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA}}^{\mathrm{GAO}}} \cdot X_{\mathrm{GAO}}$
26. Aerobic storage of GLY	$q_{\mathrm{GLY}}^{\mathrm{GAO}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA\_GLY}}^{\mathrm{GAO}}} \cdot \frac{K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}}}{K_{\mathrm{IG}}^{\mathrm{GAO}} + (K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}})} \cdot X_{\mathrm{GAO}}$
27. Anoxic (NO_2) growth	$\mu_{\mathrm{GAO}} \cdot \eta_{\mathrm{GAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{GAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA}}^{\mathrm{GAO}}} \cdot X_{\mathrm{GAO}}$
28. Anoxic (NO_2) storage of GLY	$q_{\mathrm{GLY}}^{\mathrm{GAO}} \cdot \eta_{\mathrm{GAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{GAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + K_{\mathrm{NO2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO2}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA\_GLY}}^{\mathrm{GAO}}} \cdot \frac{K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}}}{K_{\mathrm{IG}}^{\mathrm{GAO}} + (K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}})} \cdot X_{\mathrm{GAO}}$
29. Anoxic (NO_3) growth	$\mu_{\mathrm{GAO}} \cdot \eta_{\mathrm{GAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{GAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA}}^{\mathrm{GAO}}} \cdot X_{\mathrm{GAO}}$
30. Anoxic (NO_3) storage of GLY	$q_{\mathrm{GLY}}^{\mathrm{GAO}} \cdot \eta_{\mathrm{GAO}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{GAO}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{GAO}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO2}} + S_{\mathrm{NO3}}} \cdot \frac{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}}}{X_{\mathrm{PHA,G}} / X_{\mathrm{GAO}} + K_{\mathrm{PHA\_GLY}}^{\mathrm{GAO}}} \cdot \frac{K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}}}{K_{\mathrm{IG}}^{\mathrm{GAO}} + (K_{\mathrm{MG}}^{\mathrm{GAO}} - X_{\mathrm{GLY,G}} / X_{\mathrm{GAO}})} \cdot X_{\mathrm{GAO}}$
31. Lysis of GAO	$b_{\mathrm{GAO}} \cdot X_{\mathrm{GAO}}$
32. Lysis of PHA	$b_{\mathrm{PHA}} \cdot X_{\mathrm{PHA,G}}$
33. Lysis of GLY	$b_{\mathrm{GLY}} \cdot X_{\mathrm{GLY,G}}$

Hydrolysis

34. Aerobic hydrolysis	$k_{\mathrm{h}} \cdot \frac{S_{\mathrm{O2}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{h}}} \cdot \frac{X_{\mathrm{S}} / X_{\mathrm{Het}}}{X_{\mathrm{S}} / X_{\mathrm{Het}} + K_{\mathrm{X}}} \cdot X_{\mathrm{Het}}$
35. Anoxic hydrolysis	$k_{\mathrm{h}} \cdot \eta_{\mathrm{NO3\_h}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{h}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{h}}} \cdot \frac{S_{\mathrm{NO3}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{h}}} \cdot \frac{X_{\mathrm{S}} / X_{\mathrm{Het}}}{X_{\mathrm{S}} / X_{\mathrm{Het}} + K_{\mathrm{X}}} \cdot X_{\mathrm{Het}}$
36. Anaerobic hydrolysis	$k_{\mathrm{h}} \cdot \eta_{\mathrm{fe}} \cdot \frac{K_{\mathrm{O2}}^{\mathrm{h}}}{S_{\mathrm{O2}} + K_{\mathrm{O2}}^{\mathrm{h}}} \cdot \frac{K_{\mathrm{NO3}}^{\mathrm{h}}}{S_{\mathrm{NO3}} + K_{\mathrm{NO3}}^{\mathrm{h}}} \cdot \frac{X_{\mathrm{S}} / X_{\mathrm{Het}}}{X_{\mathrm{S}} / X_{\mathrm{Het}} + K_{\mathrm{X}}} \cdot X_{\mathrm{Het}}$

Supplementary Table III. Stoichiometric parameters for microbial reactions

Description	Symbol	Unit	Value	Reference
Ammonia-oxidizing bacteria (AOB)				
Yield of biomass on substrate	Y_{AOB}	$g_{COD}\ g_{N}^{-1}$	0.4	Henze et al., 2000
Nitrite-oxidizing bacteria (NOB)				
Yield of biomass on substrate	Y_{NOB}	$g_{COD}\ g_{N}^{-1}$	0.3	Henze et al., 2000
Heterotrophic bacteria (Het)				
Yield of biomass on substrate	Y_{Het}	$g_{COD}\ g_{COD}^{-1}$	0.625	Henze et al., 2000
Polyphosphate accumulating organisms (PAO)				
Acetate requirement for PHA storage	$Y_{S\_A}^{PAO}$	$g_{COD}\ g_{COD}^{-1}$	0.77	Yagci et al., 2004
PP requirement for PHA storage	Y_{PO4}^{PAO}	$g_{P}\ g_{COD}^{-1}$	0.41	Yagci et al., 2004
PHA requirement for PP storage	Y_{PHA}^{PAO}	$g_{COD}\ g_{COD}^{-1}$	0.2	Henze et al., 2000
Yield of biomass on substrate	Y_{PAO}	$g_{COD}\ g_{COD}^{-1}$	0.625	Henze et al., 2000
Glycogen yield coefficient	Y_{GLY}^{PAO}	$g_{COD}\ g_{COD}^{-1}$	1.0	Yagci et al., 2004
Glycogen accumulating organisms (GAO)				
Acetate requirement for PHA storage	$Y_{S\_A}^{GAO}$	$g_{COD}\ g_{COD}^{-1}$	0.46	Yagci et al., 2004
Yield of biomass on substrate	Y_{GAO}	$g_{COD}\ g_{COD}^{-1}$	0.625	Yagci et al., 2004
Glycogen yield coefficient	Y_{GLY}^{GAO}	$g_{COD}\ g_{COD}^{-1}$	1.0	Yagci et al., 2004
Others				
Fraction of X_I	f_{XI}	$g_{COD}\ g_{COD}^{-1}$	0.1	Henze et al., 2000

Supplementary Table IV. Kinetic parameters for microbial reactions

Description	Symbol	Unit	Value	Reference
Ammonia-oxidizing bacteria (AOB)				
Maximum specific growth rate	μ_{AOB}	day^{-1}	2.0	Adapted from de Kreuk et al., 2007
Rate of lysis	b_{AOB}	day^{-1}	0.1	de Kreuk et al., 2007
O_2 half-saturation coefficient	K_{O2}^{AOB}	g_{O2} m^{-3}	0.01	Adapted from de Kreuk et al., 2007
NH_4^+ half-saturation coefficient	K_{NH4}^{AOB}	g_N m^{-3}	1.1	Adapted from de Kreuk et al., 2007
Nitrite-oxidizing bacteria (NOB)				
Maximum specific growth rate	μ_{NOB}	day^{-1}	1.0	Adapted from de Kreuk et al., 2007
Rate of lysis	b_{NOB}	day^{-1}	0.06	de Kreuk et al., 2007
O_2 half-saturation coefficient	K_{O2}^{NOB}	g_{O2} m^{-3}	0.2	Adapted from de Kreuk et al., 2007
NO_2^- half-saturation coefficient	K_{NO2}^{NOB}	g_N m^{-3}	0.8	Adapted from de Kreuk et al., 2007
Heterotrophic bacteria (Het)				
Maximum specific growth rate	μ_{Het}	day^{-1}	6.0	Henze et al., 2000
Anoxic reduction factor for μ_{Het}	η_{Het}	–	0.8	Henze et al., 2000
Rate of lysis	b_{Het}	day^{-1}	0.4	Henze et al., 2000
O_2 half-saturation coefficient	K_{O2}^{Het}	g_{O2} m^{-3}	0.2	Henze et al., 2000
NO_2^- half-saturation coefficient	K_{NO2}^{Het}	g_N m^{-3}	0.5	Assumed in this study
NO_3^- half-saturation coefficient	K_{NO3}^{Het}	g_N m^{-3}	0.5	Henze et al., 2000
S_F half-saturation coefficient	$K_{S\_F}^{Het}$	g_{COD} m^{-3}	4.0	Henze et al., 2000
Acetate half-saturation coefficient	$K_{S\_A}^{Het}$	g_{COD} m^{-3}	4.0	Henze et al., 2000
Maximum specific fermentation rate	q_{fe}	g_{S_F} $g_{X\_H}^{-1}$ day^{-1}	1.0	Adapted from Henze et al., 2000
Polyphosphate accumulating organisms (PAO)				
Rate constant for PHA storage	q_{PHA}^{PAO}	g_{COD} g_{COD}^{-1} day^{-1}	3.4	Yagci et al., 2004
Rate constant for PP storage	q_{PP}^{PAO}	g_{COD} g_{COD}^{-1} day^{-1}	2.0	Yagci et al., 2004
Maximum specific growth rate	μ_{PAO}	day^{-1}	1.0	Yagci et al., 2004
Rate constant for GLY storage	q_{GLY}^{PAO}	g_{COD} g_{COD}^{-1} day^{-1}	2.7	Yagci et al., 2004
Anoxic reduction factor for μ_{PAO}	η_{PAO}	–	0.6	Henze et al., 2000
Rate of lysis of PAO	b_{PAO}	day^{-1}	0.02	Adapted from Henze et al., 2000
Rate of lysis of PP	b_{PP}	day^{-1}	0.02	Adapted from Henze et al., 2000
Rate of lysis of PHA	b_{PHA}^{PAO}	day^{-1}	0.02	Adapted from Henze et al., 2000
Rate of lysis of GLY	b_{GLY}	day^{-1}	0.02	Adapted from Henze et al., 2000
O_2 half-saturation coefficient	K_{O2}^{PAO}	g_{O2} m^{-3}	0.2	Henze et al., 2000
NO_2^- half-saturation coefficient	K_{NO2}^{PAO}	g_N m^{-3}	0.5	Assumed in this study
Acetate half-saturation coefficient	$K_{S\_A}^{PAO}$	g_{COD} m^{-3}	4.0	Henze et al., 2000
Poly-P half-saturation coefficient	K_{PP}^{PAO}	g_{X_PP} $g_{X\_PAO}^{-1}$ m^{-3}	0.01	Henze et al., 2000
Glycogen half-saturation coefficient	K_{GLY}^{PAO}	g_{X_GLY} $g_{X\_PAO}^{-1}$ m^{-3}	0.001	Yagci et al., 2004
Phosphorus half-saturation coefficient	K_{PO4}^{PAO}	g_P m^{-3}	0.5	Yagci et al., 2004
PHA for PP storage half-saturation coefficient	$K_{PHA\_PP}^{PAO}$	g_{X_PHA} $g_{X\_PAO}^{-1}$ m^{-3}	0.05	Yagci et al., 2004
Maximum ratio of X_{PP}/X_{PAO}	K_{MP}^{PAO}	g_{X_PP} $g_{X\_PAO}^{-1}$ m^{-3}	0.34	Henze et al., 2000
Polyphosphate storage inhibition coefficient	K_{IP}^{PAO}	g_{X_PP} $g_{X\_PAO}^{-1}$ m^{-3}	0.02	Henze et al., 2000
PHA for growth half-saturation coefficient	K_{PHA}^{PAO}	g_{X_PHA} $g_{X\_PAO}^{-1}$ m^{-3}	0.05	Yagci et al., 2004
PHA for glycogen storage half-saturation coefficient	$K_{PHA\_GLY}^{PAO}$	g_{X_PHA} $g_{X\_PAO}^{-1}$ m^{-3}	0.01	Yagci et al., 2004
Maximum ratio of X_{GLY}/X_{PAO}	K_{MG}^{PAO}	g_{X_GLY} $g_{X\_PAO}^{-1}$ m^{-3}	0.15	Yagci et al., 2004
Glycogen storage inhibition coefficient	K_{IG}^{PAO}	g_{X_GLY} $g_{X\_PAO}^{-1}$ m^{-3}	0.02	Yagci et al., 2004
Glycogen accumulating organisms (GAO)				
Rate constant for PHA storage	q_{PHA}^{GAO}	g_{COD} g_{COD}^{-1} day^{-1}	3.0	Yagci et al., 2004
Rate constant for GLY storage	q_{GLY}^{GAO}	g_{COD} g_{COD}^{-1} day^{-1}	2.7	Yagci et al., 2004
Maximum specific growth rate	μ_{GAO}	day^{-1}	1.0	Yagci et al., 2004
Anoxic reduction factor for μ_{GAO}	η_{GAO}	–	0.6	Assumed in this study
Rate of lysis of GAO	b_{GAO}	day^{-1}	0.01	Adapted from Yagci et al., 2004
Rate of lysis of PHA	b_{PHA}^{GAO}	day^{-1}	0.01	Adapted from Yagci et al., 2004
Rate of lysis of GLY	b_{GLY}	day^{-1}	0.01	Adapted from Yagci et al., 2004
O_2 half-saturation coefficient	K_{O2}^{GAO}	g_{O2} m^{-3}	0.2	Manga et al., 2001
NO_2^- half-saturation coefficient	K_{NO2}^{GAO}	g_N m^{-3}	0.5	Assumed in this study
NO_3^- half-saturation coefficient	K_{NO3}^{GAO}	g_N m^{-3}	0.5	Manga et al., 2001
Glycogen half-saturation coefficient	K_{GLY}^{GAO}	g_{X_GLY} $g_{X\_GAO}^{-1}$ m^{-3}	0.001	Yagci et al., 2004
PHA for growth half-saturation coefficient	K_{PHA}^{GAO}	g_{X_PHA} $g_{X\_GAO}^{-1}$ m^{-3}	0.01	Yagci et al., 2004
PHA for glycogen storage half-saturation coefficient	K_{GLY}^{GAO}	g_{X_PHA} $g_{X\_GAO}^{-1}$ m^{-3}	0.01	Yagci et al., 2004
Maximum ratio of X_{GLY}/X_{GAO}	K_{MG}^{GAO}	g_{X_GLY} $g_{X\_GAO}^{-1}$ m^{-3}	0.3	Yagci et al., 2004
Glycogen storage inhibition coefficient	K_{IG}^{GAO}	g_{X_GLY} $g_{X\_GAO}^{-1}$ m^{-3}	0.02	Yagci et al., 2004
Hydrolysis				
Hydrolysis rate constant	k_h	day^{-1}	1.0	Adapted from Henze et al., 2000
Anoxic hydrolysis reduction coefficient	η_{NO3_h}	–	0.6	Henze et al., 2000
Anaerobic hydrolysis reduction coefficient	η_{fe}	–	0.4	Henze et al., 2000
Hydrolysis saturation constant for O_2	K_{O2}^{h}	g_{O2} m^{-3}	0.2	Henze et al., 2000
Hydrolysis saturation constant for particulate COD	K_X	g_{X_S} m^{-3}	0.1	Henze et al., 2000
Hydrolysis saturation constant for NO_3	K_{NO3}^{h}	g_N m^{-3}	0.5	Henze et al., 2000

Supplementary Table V. Other parameters used in the simulation

Description	Symbol	Unit	Value	Reference
Diffusivity of O_2 in water	D_{O2}	m^2 day^{-1}	2.0×10^{-4}	Xavier et al., 2007
Diffusivity of NH_4^+ in water	D_{NH4}	m^2 day^{-1}	1.7×10^{-4}	Xavier et al., 2007
Diffusivity of NO_2^- in water	D_{NO2}	m^2 day^{-1}	1.6×10^{-4}	Xavier et al., 2007
Diffusivity of NO_3^- in water	D_{NO3}	m^2 day^{-1}	1.6×10^{-4}	Xavier et al., 2007
Diffusivity of PO_4^{3-} in water	D_{PO4}	m^2 day^{-1}	1.1×10^{-4}	Xavier et al., 2007
Diffusivity of S_F in water	D_{S_F}	m^2 day^{-1}	9.6×10^{-5}	Xavier et al., 2007
Diffusivity of S_A in water	D_{S_A}	m^2 day^{-1}	9.6×10^{-5}	Xavier et al., 2007
Boundary layer thickness	L_L	μm	25	Assumed in this study
Specific mass of active and inert biomass	ρ_X	$g_{COD,X}$ m^{-3}	350,000	de Kreuk et al., 2007
Specific mass of PHA	ρ_{PHA}	$g_{COD,E}$ m^{-3}	1×10^{8}	de Kreuk et al., 2007 [a]
Reactor volume	V	m^3	1×10^{-5}	Assumed in this study

[a] A high value of ρ_{PHA} was assumed to make the volume of storage particulate components negligible compared with the active biomass.

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