Electronic Supplementary Material (ESI) for Environmental Science: Water Research & Technology.

Supporting information

Functional guild dynamics in a single-sludge shortcut nitrogen and phosphorus removal reactor: a modeling study

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1 model set-up and functional guilds calcaulation

Functional guilds including AOB, NOB, PAOs, and DPAOs were quantified with rate equations and parameter values from Simba# inCTRL ASM matrix as shown below:

Net specific growth rate of AOB (d^{-1}) = μ_{AOB} =

$$\hat{\mu}_{AOB}\frac{S_{NHx}}{S_{NHx}+K_{NHx,AOB}}\frac{S_{O2}}{S_{O2}+K_{O2,AOB}}\frac{S_{PO4}}{S_{PO4}+K_{PO4,ANB}}\frac{S_{ALK}}{S_{ALK}+K_{ALK,AOB}}-b_{AOB,O2}\frac{S_{O2}}{S_{O2}+K_{O2,AOB}}$$
$$-b_{AOB,NOx}\frac{S_{NO2}+S_{NO3}}{S_{NO2}+S_{NO3}+K_{NOx,ANB}}\frac{K_{O2,AOB}}{S_{O2}+K_{O2,AOB}}-b_{AOB,ANA}$$
$$\frac{K_{NOx,AOB}}{S_{NO2}+S_{NO3}+K_{NOx,ANB}}\frac{K_{O2,AOB}}{S_{O2}+K_{O2,AOB}}$$

Where:

$\hat{\mu}_{AOB}$ = maximum specific growth rate of AOB (d^{-1})=0.9

S_{NHx} = concentration of NH_4^+ + NH_3 (mgN/L)

$K_{NHx,AOB}$ = AOB half saturation coefficient for (NH_4^+ + NH_3) (mgN/L)=0.7

S_{O2} = concentration of dissolved O_2 (mgO_2/L)

$K_{O2,AOB}$ = AOB half saturation coefficient for dissolved O_2 (mgO_2/L)=0.25

S_{PO4} = concentration of dissolved PO_4^{3-} (mgP/L)

$K_{PO4,ANB}$ = nitrifier nutrient half saturation coefficient for PO_4^{3-} (mgP/L)=0.001

S_{ALK} = concentration of alkalinity (meq/L)

$K_{ALK,AOB}$ = AOB half saturation coefficient for alkalinity (meq/L)=0.5

$b_{AOB,O2}$ = maximum specific aerobic decay rate of AOB (d^{-1})=0.17

$b_{AOB,NOx}$ = maximum specific anoxic decay rate of AOB (d^{-1})=0.1

S_{NO3} = concentration of dissolved NO_3^- (mgN/L)

S_{NO2} = concentration of dissolved NO_2^- (mgN/L)

$K_{NOx,ANO}$ = nitrifier half saturation for anoxic conditions (mgN/L)=0.03

$b_{AOB,ANA}$ = maximum specific anaerobic decay rate of AOB (d^{-1})=0.05

Net specific growth rate of NOB (d^{-1}) = μ_{NOB} =

$$\hat{\mu}_{NOB}\frac{S_{NO2}}{S_{NO2}+K_{NO2,NOB}}\frac{S_{O2}}{S_{O2}+K_{O2,NOB}}\frac{S_{NHx}}{S_{NHx}+K_{NHx,ANB}}\frac{S_{PO4}}{S_{PO4}+K_{PO4,ANB}}\frac{S_{ALK}}{S_{ALK}+K_{ALK,AOB}}-b_{NOB,O2}\frac{S_{O2}}{S_{O2}+K_{O2,NOB}}-b_{NOB,NOx}\frac{S_{NO2}+S_{NO3}}{S_{NO2}+S_{NO3}+K_{NOx,ANB}}\frac{K_{O2,NOB}}{S_{O2}+K_{O2,NOB}}-b_{NOB,ANA}\frac{K_{NOx,AOB}}{S_{NO2}+S_{NO3}+K_{NOx,ANB}}\frac{K_{O2,NOB}}{S_{O2}+K_{O2,NOB}}$$

Where:

$\hat{\mu}_{NOB}$ = maximum specific growth rate of NOB (d^{-1})=0.7

$K_{NO2,NOB}$ = NOB half saturation coefficient for NO_2^- (mgN/L)=0.1

$K_{O2,NOB}$ = NOB half saturation coefficient for dissolved O_2 (mgO_2/L)=0.1

$K_{NHx,ANB}$ = nitrifier nutrient half saturation coefficient for $(NH_4^+ + NH_3)^-$ (mgN/L)=0.001

$K_{ALK,NOB}$ = NOB half saturation coefficient for alkalinity (meq/L)=0.5

$b_{NOB,O2}$ = maximum specific aerobic decay rate of NOB (d^{-1})=0.15

$b_{NOB,NOx}$ = maximum specific anoxic decay rate of NOB (d^{-1})=0.07

$b_{NOB,ANA}$ = maximum specific anaerobic decay rate of NOB (d^{-1})=0.04

Specific growth rate of PAOs on PHA and O_2 (d^{-1}) = $\mu_{PAO,O2}$ =

$$\hat{\mu}_{PAO}\frac{\frac{X_{PHA}}{X_{PAO}}}{\frac{X_{PHA}}{X_{PAO}}+K_{PHA}}\frac{S_{O2}}{S_{O2}+K_{O2,OHO}}\frac{S_{NHx}}{S_{NHx}+K_{NHx,OHO}}\frac{S_{PO4}}{S_{PO4}+K_{PO4,PAO}}\frac{S_{ALK}}{S_{ALK}+K_{ALK}}$$

Where:

$\hat{\mu}_{PAO} =$ maximum specific growth rate of PAOs (d^{-1})=0.95

$X_{PHA} =$ concentration of polyhydroxyalkanonates-PHAs (mgCOD/L)

$X_{PAO} =$ concentration of PAOs (mgCOD/L)

$K_{PHA} =$ half saturation coefficient for PHA (mgCOD/L) =0.1

$K_{O2,OHO} = OHO\ and\ PAO$ half saturation coefficient for dissolved O_2 (mgO_2/L) =0.05

$K_{NHx,OHO} = OHO\ and\ PAO$ nutrient half saturation coefficient for ($NH_3+NH_4^+$) (mgN/L) =0.001

$K_{PO4,PAO} = PAO$ half saturation coefficient for PO_4^{3-} (mgP/L) =0.15

$K_{ALK} = PAO$ half saturation coefficient for alkalinity (mgN/L) =0.1

Specific growth rate of PAOs on PHA and NO_2^- (d^{-1}) = $\mu_{PAO,NO2}$ =

$$\hat{\mu}_{PAO}\eta_{anox,PAO}\frac{\frac{X_{PHA}}{X_{PAO}}}{\frac{X_{PHA}}{X_{PAO}}+K_{PHA}}\frac{S_{NO2}}{S_{NO2}+K_{NO2,OHO}}\frac{K_{O2,OHO}}{S_{O2}+K_{O2,OHO}}\frac{S_{NHx}}{S_{NHx}+K_{NHx,OHO}}\frac{S_{PO4}}{S_{PO4}+K_{PO4,PAO}}\frac{S_{ALK}}{S_{ALK}+K_{ALK}}$$

Where:

$\eta_{anox,PAO}$=PAO anoxic growth factor=0.33

$K_{NO2,OHO} = PAO\ and\ OHO$ half saturation coefficient for NO_2^- (mgN/L) =0.05

Specific growth rate of PAOs on PHA and NO_3^- (d^{-1}) = $\mu_{PAO,NO3}$ =

$$\hat{\mu}_{PAO}\eta_{anox,PAO}\frac{\frac{X_{PHA}}{X_{PAO}}}{\frac{X_{PHA}}{X_{PAO}}+K_{PHA}}\frac{S_{NO3}}{S_{NO3}+K_{NO3,OHO}}\frac{K_{NO2,OHO}}{S_{NO2}+K_{NO2,OHO}}\frac{K_{O2,OHO}}{S_{O2}+K_{O2,OHO}}\frac{S_{NHx}}{S_{NHx}+K_{NHx,OHO}}\frac{S_{PO4}}{S_{PO4}+K_{PO4,PAO}}\frac{S_{ALK}}{S_{ALK}+K_{ALK}}$$

Where:

$K_{NO3,OHO} = PAO\ and\ PAO$ half saturation coefficient for NO_3^- (mgN/L) =0.1

Specific PHA storage rate from VFAs by PAOs (d^{-1}):=

$$q_{PAO,PHA}\frac{\frac{X_{PP,LO}}{X_{PAO}}}{\frac{X_{PP,LO}}{X_{PAO}}+K_{PP,LO}}\frac{S_{VFA}}{S_{VFA}+K_{STORE,VFA}}\frac{S_{ALK}}{S_{ALK}+K_{ALK}}$$

Where:

$q_{PAO,PHA}$= PHA storage rate by PAOs (d^{-1}) =6

$K_{PP,LO}$ = polyphosphate half saturation for storage (mgP/mgCOD)=0.01

S_{VFA} = concentration of volatile fatty acids (mgCOD/L)

$K_{STORE,VFA}$ = VFA half saturation for storage (mgCOD/L)=1

2 Ammonium oxidation rate under various scenarios

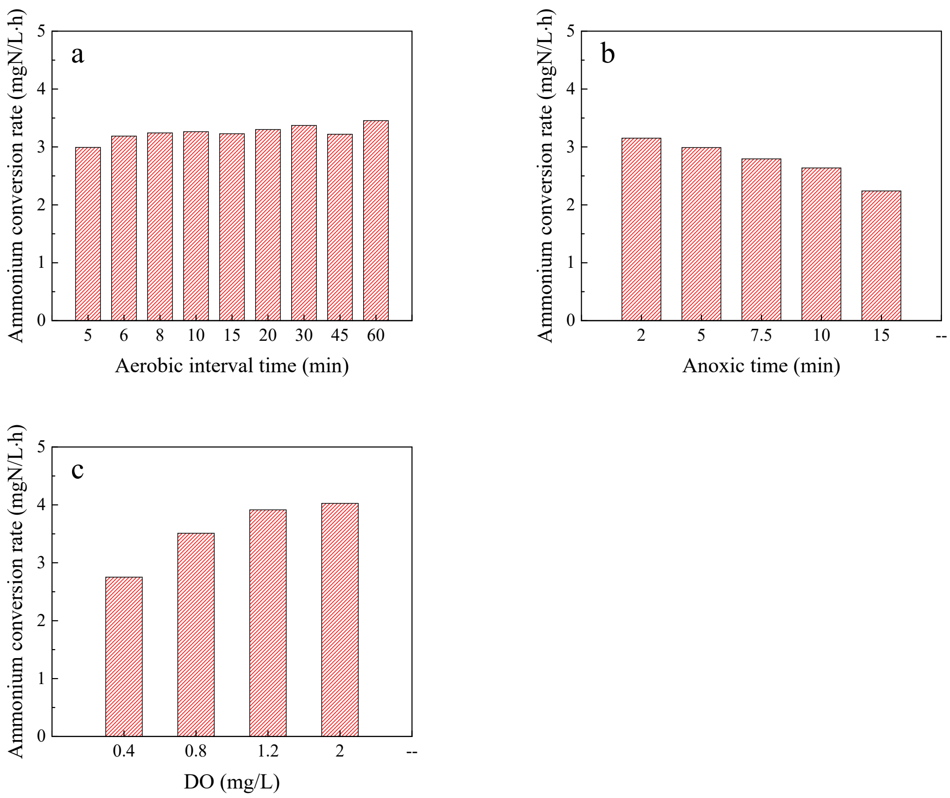

Figure S1. Ammonium oxidation rate under various scenarios