Supporting Information:

Operational boundaries for nitrite accumulation in nitrification based on minimum/maximum substrate concentrations that include effects of oxygen limitation, pH, and free ammonia and free nitrous acid inhibition

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Section S1: Derivation of the equation of minimum substrate concentration curve

The derivation of the general MSC equation follows the steps of the traditional S_{min} derivation. First, the mass balance of biomass in a continuous flow reactor is shown in eq. A1

$$\underbrace{\frac{dX}{dt}\cdot V}_{\text{Accumulation rate}} = \underbrace{Q_{in}\cdot X^{\circ} - Q_{out}\cdot X_a}_{\text{Advection rate of biomass}} + \underbrace{Y\cdot\hat{q}\cdot\frac{S_{E.D}}{(K_{E.D}+S_{E.D})}\cdot\frac{S_{E.A}}{(S_{E.A}+S_{E.A})}\cdot X_a\cdot V - b\cdot X_a\cdot V}_{\text{Biological growth and decay rate}} \tag{A1}$$

If the system is at steady-state and influent flow flow rate is equal to effluent flow rate, eq. A1 transforms to eq. A2.

$$0 = Q\cdot X^{\circ} - Q\cdot X_a + Y\cdot\hat{q}\cdot\frac{S_{E.D}}{(K_{E.D}+S_{E.D})}\cdot\frac{S_{E.A}}{(S_{E.A}+S_{E.A})}\cdot X_a\cdot V - b\cdot X_a\cdot V \tag{A2}$$

Dividing by active biomass concentration, X_a and flow rate, Q, converts eq. A2 to eq. A3.

$$0 = \frac{X^{\circ}}{X_a} - 1 + Y\cdot\hat{q}\cdot\frac{S_{E.D}}{(K_{E.D}+S_{E.D})}\cdot\frac{S_{E.A}}{(S_{E.A}+S_{E.A})}\cdot\frac{V}{Q} - b\cdot\frac{V}{Q} \tag{A3}$$

Since V/Q can be defined as the hydraulic retention time (HRT, θ), eq. A3 can be rewritten as eq. A4.

$$0 = \frac{X^{\circ}}{X_a} - 1 + Y\cdot\hat{q}\cdot\frac{S_{E.D}}{(K_{E.D}+S_{E.D})}\cdot\frac{S_{E.A}}{(S_{E.A}+S_{E.A})}\cdot\theta - b\cdot\theta \tag{A4}$$

The definition of S_{min} in this system is the concentration at infinitely large HRT. Letting θ go to infinity converts eq. A4 to eq. A5a for $S_{D,min}$ and eqn.A5b, for $S_{A,min}$. Eqns. 3a and 3b in the main text are the same as eqns A5a and A5b.

$$0 = Y\cdot\hat{q}\cdot\frac{S_{D,min}}{(K_{E.D}+S_{D.min})}\cdot\frac{S_{E.A}}{(K_{E.A}+S_{E.A})} - b \tag{A5a}$$

$$0 = Y\cdot\hat{q}\cdot\frac{S_{E.D}}{(K_{E.D}+S_{E.D})}\cdot\frac{S_{A,min}}{(K_{E.A}+S_{A,min})} - b \tag{A5b}$$

Section S2: Derivation of minimum electron donor-substrate concentration curve with FA and FNA inhibition

The general eq. A5a in Section S1 can be expanded to eq. B1 by adding the inhibition terms for FA and FNA.

$$0 = Y \cdot \hat{q} \cdot \frac{S_{D,min}}{[K_{E.D} \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,i}}) + S_{D,min} \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,i}} + \frac{I_{FA}}{K_{I,FA,i}})]} \cdot \frac{S_{E.A}}{(K_{E.A} + S_{E.A})} - b \qquad \text{B1}$$

Eq. B1 give eq. B2a for AOB. Since S_{FA} depends on the total concentration of ammonium-N and pH (eqns. 7a and 7b), the formula of $S_{D,min}$ (which is total ammonium N) includes $f(pH) \cdot S_{D,min}$ as eqn. B2a.

$$0 = Y \cdot \hat{q} \cdot \frac{S_{D,min}}{[K_{E.D} \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}}) + S_{D,min} \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}} + \frac{f_{FA}(pH) \cdot S_{D,min}}{K_{I,FA,AOB}})]} \cdot \frac{S_{E.A}}{K_{E.A} + S_{E.A}} - b$$

B2a

Eq. B2a can be solved for $S_{D.min}$ using a quadratic equation and the quadratic formula, Eqn. B2b.

$$0 = S_{D,min}^2 \cdot b \cdot \frac{f_{FA}(pH)}{K_{I,FA,AOB}} + [b \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}}) - Y \cdot \hat{q} \cdot \frac{S_{E.A}}{K_{E.A} + S_{E.A}}] \cdot S_{D,min} + b \cdot K_{E.D} \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}})$$

$$S_{D,min} = \frac{-Z_{AOB} \pm \sqrt{Z_{AOB}{}^2 - 4 \cdot K_{E.D} \cdot \frac{f_{FA}(pH)}{K_{I,FA,AOB}} \cdot b^2 \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}})}}{2 \cdot \frac{f_{FA}(pH)}{K_{I,FA,AOB}} \cdot b} \qquad \text{B2b}$$

in which

$$Z_{AOB} = b \cdot (1 + \frac{I_{FNA}}{K_{I,FNA,AOB}}) - Y \cdot \hat{q} \cdot \frac{S_{E.A}}{(K_{E.A} + S_{E.A})}, \quad f_{FA}(pH) = \frac{17}{14} \frac{10^{pH}}{[\exp(6334/(273 + {}^{\circ}C)) + 10^{pH}]}$$

Similarly, for NOB, eq. B1 give eq. B3a

$$0 = Y \cdot \hat{q} \cdot \frac{S_{D,min}}{[K_{E.D} \cdot (1 + \frac{f_{FNA}(pH) \cdot S_{D.min}}{K_{I,FNA,NOB}}) + S_{D,min} \cdot (1 + \frac{f_{FNA}(pH) \cdot S_{D.min}}{K_{I,FNA,NOB}} + \frac{I_{FA}}{K_{I,FA,NOB}})]} \cdot \frac{S_{E.A}}{(K_{E.A} + S_{E.A})} - b$$

B3a

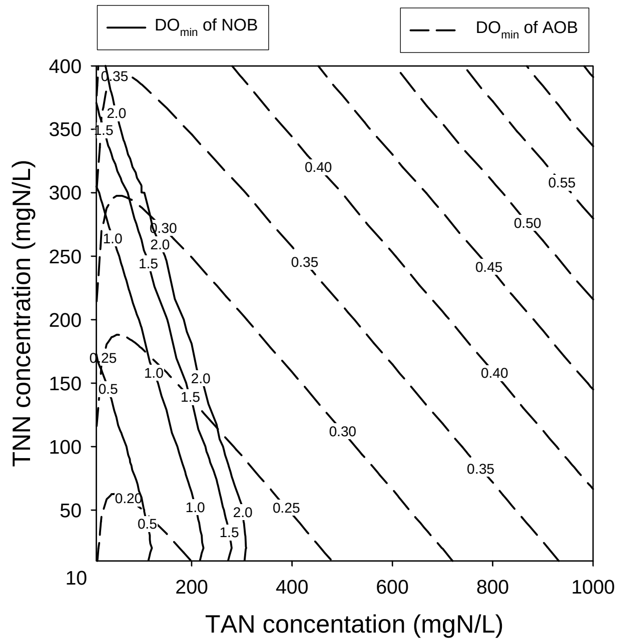
$$0 = S_{D,min}^2 \cdot b \cdot \frac{f_{FNA}(pH)}{K_{I,FNA,NOB}} + [b \cdot (1 + \frac{I_{FA}}{K_{I,FA,NOB}} + f_{FNA}(pH) \cdot \frac{K_{E.D}}{K_{I,FA,NOB}}) - Y \cdot \hat{q} \cdot \frac{S_{E.A}}{K_{E.A} + S_{E.A}}] \cdot S_{D,min} + b \cdot K_{E.D}$$

$$S_{D,min} = \frac{-Z_{NOB} \pm \sqrt{{Z_{NOB}}^2 - 4 \cdot K_{E.D} \cdot \frac{f_{FNA}(pH)}{K_{I,FNA,NOB}} \cdot b^2}}{2 \cdot \frac{f_{FNA}(pH)}{K_{I,FNA,NOB}} \cdot b}$$

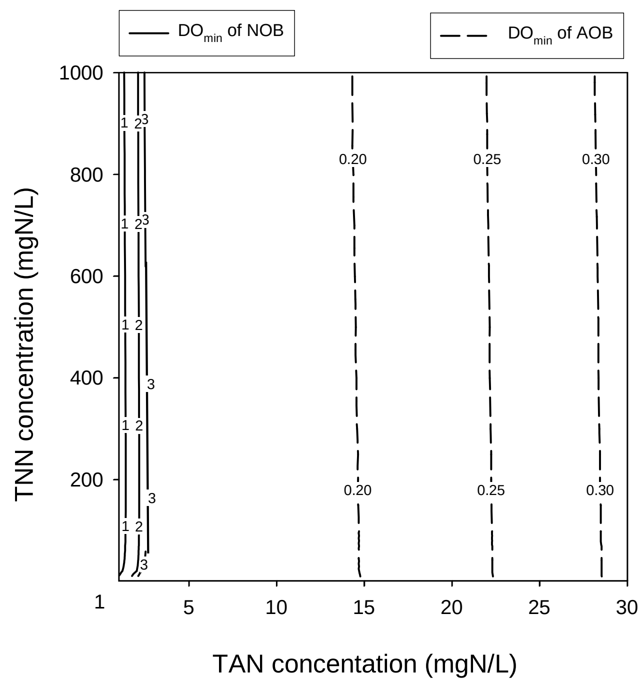
B3b

$$Z_{NOB} = b \cdot (1 + \frac{I_{FA}}{K_{I,FA,NOB}} + \frac{f_{FNA}(pH) \cdot K_{E.D}}{K_{I,FNA,NOB}}) - Y \cdot \hat{q} \cdot \frac{S_{E.A}}{(K_{E.A} + S_{E.A})}, \; f_{FNA}(pH) = \frac{47}{14} \frac{1}{[\exp(-2300/(273 + {}^{\circ}C)) \times 10^{pH}] + 1}$$

Here, since the root has the plus and minus sign, $S_{D,min}$ has two value. We define the smaller value, $S_{D,min}$ and the larger value, $S_{D,max}$ in MSC curve. Finally, we get the eqs. 6b and 6c for each AOB and NOB, respectively. By the eqs. 6b and 6c, we also get Figure S1 that shows the contour at pH 7 and pH 9.



a) pH 7



b) pH 9

Figure S1. Contour of MSC curve between TAN and TNN concentration at pH 7 and 9. The values on the line are DO_{min}.