Supplementary Material

An improved ASM-GDA approach to evaluate the production kinetics of loosely bound and tightly bound extracellular polymeric substances in biological phosphorus removal process

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1. Sensitive analysis

According to previous studies [1], the normalised sensitivity coefficient ($\delta_{i,j}$) is defined as a ratio of the percentage change in the output variable (y_i) to a 10% change in the input variable (x_j). Through sensitive analysis, a small variation in the value of a parameter (x_j) with high sensitivity will cause a large variation in the response predicted by the model. In this study, a 50% increase in the input variable is applied for the purpose of $\delta_{i,j}$ calculation. Through analyzing the effects of the model parameters on the extended ASM2 model outputs (S_{PO4}, X_{TB-EPS}, X_{LB-EPS}, and X_{PP}), the coefficient $\delta_{i,j}$ of the individual parameter is calculated by Eq. (S1).

$$\delta_{i,j} = \frac{x_j \Delta y_i}{y_i \Delta x_j} \qquad \text{(S1)}$$

where the vector y_i (i =1, 2, ..., n) represents the model output variables; the vector x_j (j=1, 2, ..., n) represents the independent model parameters.

For each input variable, the influence of a model parameter on the model output can be interpreted as follows: $\delta_{i,j} < 0.5$ represents that the model parameter has no significant influence on the model output; $\delta_{i,j} > 0.5$ represents that the model parameter is influential and needs calibration.

References

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Table S1 Kinetic rates expressions in the extended ASM2 model

	Process	ρ_i
1	Aerobic growth of X_H on S_S	$\mu_H \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_S}{K_S+S_S} \cdot \frac{S_{PO_4}}{K_{PO_4}+S_{PO_4}} \cdot \frac{S_{NH_4}}{K_{NH_4}+S_{NH_4}} \cdot \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \cdot X_H$
2	Aerobic growth of XH on S_{EPS}	$\mu_{S_{EPS}} \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{EPS}}{K_{EPS}+S_{EPS}} \cdot \frac{S_{PO_4}}{K_{PO_4}+S_{PO_4}} \cdot \frac{S_{NH_4}}{K_{NH_4}+S_{NH_4}} \cdot \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \cdot X_H$
3	Formation of S_{EPS} from X_{TB-EPS}	$k_{h,TB-EPS} \cdot \frac{S_S}{K_{S,S_{EPS}}+S_S} \cdot X_{TB-EPS}$
4	Formation of S_{EPS} from X_{LB-EPS}	$k_{h,LB-EPS} \cdot \frac{S_S}{K_{S,S_{EPS}}+S_S} \cdot X_{LB-EPS}$
5	Storage of X_{PHA}	$q_{PHA} \frac{S_S}{K_S+S_S} \cdot \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \cdot \frac{X_{PP}/X_{PAO}}{K_{PP}+X_{PP}/X_{PAO}} \cdot X_{PAO}$
6	Storage of X_{PP}	$q_{PP} \cdot \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{PO_4}}{K_{PO_4}+S_{PO_4}} \cdot \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}} \cdot \frac{K_{\max}-X_{PP}/X_{PAO}}{K_{IPP}+K_{\max}-X_{PP}/X_{PAO}}$
7	Decomposing of X_{PHA}	$b_{PHA} \cdot X_{PHA} \frac{S_{ALK}}{K_{ALK}+S_{ALK}}$
8	Decomposing of X_{PP}	$b_{PP} \cdot X_{PP} \frac{S_{ALK}}{K_{ALK}+S_{ALK}}$
9	Aerobic growth of X_{PAO}	$\mu_{PAO} \frac{S_{O_2}}{K_{O_2}+S_{O_2}} \cdot \frac{S_{PO_4}}{K_{PO_4}+S_{PO_4}} \cdot \frac{S_{NH_4}}{K_{NH_4}+S_{NH_4}} \cdot \frac{S_{ALK}}{K_{ALK}+S_{ALK}} \cdot \frac{X_{PHA}/X_{PAO}}{K_{PHA}+X_{PHA}/X_{PAO}} \cdot X_{PAO}$
10	Lysis of X_H	$b_H \cdot X_H$
11	Lysis of X_{PAO}	$b_{PAO} \cdot X_{PAO} \frac{S_{ALK}}{K_{ALK}+S_{ALK}}$

Table S2 Stoichiometric and kinetic model parameters for the extended ASM2 model

Parameters	Description	Value	Unit	References
Y_H	Heterotrophic yield coefficient	0.625	$g\ COD/g\ COD$	ASM2
Y_{PAO}	PAOs yield coefficient	0.625	$g\ COD/g\ COD$	ASM2
$Y_{H,S_{EPS}}$	Yield coefficient for growth on S_{EPS}	0.625	$g\ COD_x/g\ COD_{S_{EP}}$	[2,3]
Y_{PHA}	PHA requirement for storage of phosphate in the form of X_{PP}	0.20	$g\ COD/g\ COD$	ASM2
Y_{PO_4}	PP requirement for storage of X_{PHA}	0.40	$g\ P/g\ COD$	ASM2
μ_H	Maximum growth rate of heterotroph	6.00	d^{-1}	ASM2
μ_{PAO}	Maximum growth rate of PAO	1.00	d^{-1}	ASM2
$\mu_{S_{EPS}}$	Maximum rate of S_{EPS} degradation	0.0029	h^{1}	[2,3]
b_H	Decay rate of heterotroph	0.40	d^{-1}	ASM2
b_{PAO}	Decay rate of PAO	0.20	d^{-1}	ASM2
b_{PP}	Decomposition rate constants of X_{PP}	0.20	d^{-1}	ASM2
b_{PHA}	Decomposition rate constants of X_{PHA}	0.20	d^{-1}	ASM2
q_{PP}	Rate constants of PP storage	1.50	d^{-1}	ASM2
q_{PHA}	Rate constants of PHA storage	3.00	d^{-1}	ASM2
k_{TB-EPS}	TB-EPS formation coefficient	0.18	$g\ COD_{TB-EPS}/g\ C$	[2,3]
k_{LB-EPS}	LB-EPS formation coefficient	0.18	$g\ COD_{LB-EPS}/g\ C$	[2,3]
K_{O_2}	Dissolve oxygen affinity constant	0.20	$g\ O_2/m^3$	ASM2
K_s	S_s affinity constant for heterotroph	4.00	$g\ COD/m^3$	ASM2
K_{PO_4}	Affinity constant for heterotroph	0.01	$g\ P/m^3$	ASM2
K_{ALK}	Alkalinity affinity constant for heterotroph	0.10	$mol(HCO_3^-)/m^3$	ASM2
$K_{S,S_{EPS}}$	Affinity constant for S_{EPS} formation	0.02	$g\ COD_{S_{EPS}}/m$	[2,3]
$K_{S_{EPS}}$	Biomass affinity constant for S_{EPS}	85	$g\ COD_{S_{EPS}}/m$	[2,3]
$i_{P,BM}$	P contents in X_H, X_{PAO}, X_{TB-EPS}, X_{LB-EPS}	0.02	$g\ P/g\ COD$	ASM2, [4]
$k_{h,TB-EPS}$	TB-EPS hydrolysis rate constant	0.228	d^{-1}	[2,3]
$k_{h,LB-EPS}$	LB-EPS hydrolysis rate constant	0.4	d^{-1}	Extended ASM2
$f_{PP,TB-EPS}$	X_{TB-EPS} fraction during X_{PP} storage and decomposing processes	0.09	$g\ S_{PO_4}/g\ X_{TB-EPS}$	Extended ASM2
$f_{PP,LB-EPS}$	X_{LB-EPS} fraction during X_{PP} storage and decomposing processes	0.04	$g\ S_{PO_4}/g\ X_{LB-EPS}$	Extended ASM2

Table S3 Stoichiometric matrix for the extended ASM2 model

	Process	S_O	S_s	S_{PO_4}	S_{NH_4}	S_{ALK}	S_{EPS}	X_{TB-EPS}	X_{LB-EPS}	X_H	X_I	X_S	X_{PAO}	X_{PP}	X_{PHA}
1	Aerobic growth of X_H on S_S	$-\frac{[1-k_{TB-EPS}-k_{TB-EPS}]}{Y_H}$	$-\frac{1}{Y_H}$	$-[i_{P,X_{TB-EPS}}\cdot\frac{k_{TB-EF}}{Y_H}$				$\frac{k_{TB-EPS}}{Y_H}$	$\frac{k_{LB-EPS}}{Y_H}$	$1-k_{TB-EPS}$					
2	Aerobic growth of X_H on S_{EPS}	$-\frac{1-Y_{H,S_{EPS}}}{Y_{H,S_{EPS}}}$		v_{2,PO_4}			$-\frac{1}{Y_{H,S_{EPS}}}$			1					
3	Formation of S_{EPS} from X_{TB-EPS}			v_{3,PO_4}			1	-1							
4	Formation of S_{EPS} from X_{LB-EPS}			v_{4,PO_4}			1		-1						
5	Storage of X_{PHA}		-1	Y_{PO_4}										$-Y_{PO_4}$	1
6	Storage of X_{PP}	$-Y_{PHA}$		-1				$f_{PP,TB-EPS}$	$f_{PP,LB-EPS}$					$1-f_{PP,TB-EP.}$	$-Y_{PHA}$
7	Decomposing of X_{PHA}		1												-1
8	Decomposing of X_{PP}			$1-f_{PP,TB-EPS}-f_{PP,L}$				$f_{PP,TB-EPS}$	$f_{PP,LB-EPS}$					-1	

9	Aerobic growth of X_{PAO}	$1-\frac{1}{Y_{PAO}}$	$-i_{P,BM}$				1	$-\frac{1}{Y_{PAO}}$
10	Lysis of X_H		v_{10,PO_4}	-1	f_{X_I}	1-f_{X_I}		
11	Lysis of X_{PAO}		v_{11,PO_4}		f_{X_I}	1-f_{X_I}	-1	