Supporting Information

Modeling Effects of H_2S on Electron Competition among Nitrogen Oxides Reduction and N_2O Accumulation during Denitrification

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Table S1. Model components

Variable	Description	Unit
S_{H2S}	H_2S concentration	(mg H_2S/L as H_2S)
S_{NO3}	Nitrate concentration	(mg N/L as NO_3^-)
S_{NO2}	Nitrite concentration	(mg N/L as NO_2^-)
S_{N2O}	Nitrous oxide concentration	(mg N/L as N_2O)
S_{N2}	Nitrogen gas concentration	(mg N/L as N_2)
S_S	COD concentration	(mg COD/L)
S_{Mred}	Reduced form of electron carrier concentration	(mmol *Mred*/(mmol biomass))
S_{Mox}	Oxidized form of electron carrier concentration	(mmol *Mred*/(mmol biomass))
X	Active heterotrophic biomass concentration	(mg COD/L)

Table S2. Kinetic and stoichiometric parameters of the developed model

Parameter	Definition	Value	Source
K_{NO2}^{H2S}	H_2S inhibition constant for nitrite reduction, R3 (mg H_2S/L)	1.56±0.11	Estimated
K_{N2O}^{H2S}	H_2S inhibition constant for N_2O reduction, R4 (mg H_2S/L)	0.088 ±0.009	Estimated
K_{NO3}^{HB}	Affinity constant for nitrate-nitrogen (mg N /L)	0.252	(1)
K_{NO2}^{HB}	Affinity constant for nitrite-nitrogen (mg N /L)	0.0574	(1)
K_{N2O}^{HB}	Affinity constant for nitrous oxide-nitrogen (mg N/L)	0.07	(2)
K_S	Affinity constant for Ss (mg COD/L)	1.6	(1)
$r_{COD,\max}$	Maximum carbon source oxidation rate (mg COD/ mg biomass COD *hour)	0.24	(2)
$r_{NO3,\max}$	Maximum nitrate reduction rate (mg N/mg biomass COD *hour)	0.0277	(2)
$r_{NO2,\max}$	Maximum nitrite reduction rate (mg N/mg biomass COD *hour)	0.0364	(2)
$r_{N2O,\max}$	Maximum nitrous oxide reaction rate (mg N/mg biomass COD *hour)	0.283	(2)
K_{Mox}	Affinity constant for S_{Mox}, R1 mmol/(mmol biomass)	0.0001	(2)
$K_{Mred,1}$	Affinity constant for S_{Mred}, R2 mmol/(mmol biomass)	0.0046	(2)
$K_{Mred,2}$	Affinity constant for S_{Mred}, R3 mmol/(mmol biomass)	0.00040	(2)
$K_{Mred,3}$	Affinity constant for S_{Mred}, R5 mmol/(mmol biomass)	0.0032	(2)
Y_H	Heterotrophic yield	0.5	(3)
C_{tot}	Total electron carrier concentration mmol/mmol biomass	0.01	(2)

References

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