

Modeling surface water and groundwater mixing and mixing-dependent denitrification with bedform dynamics

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Text 1. Model validation

The flume experiments of Wolke et al. (2019) were conducted to study the variation of oxygen plume in the homogeneous riverbed under different conditions of stream velocity and bedform mobile celerity. We simulated flume experiments by Wolke et al. (2019) and compared the hyporheic exchange process and oxygen spatial distribution with experimental measurements to ensure the accuracy of numerical modeling. The experiment was designed with a total of 5 operating conditions, each of which was repeated twice and labeled as Set 1 and Set 2.

Table S1. Parameters for the flume experiments of Wolke et al. (2019)

Parameter	Description	Value
U [m/s]	Stream velocity	0.16–0.37
H_d [cm]	Bedform height	1.3–1.94
u_c [m/h]	Bedform celerity	0–0.699
H [cm]	Water depth	13.7–14.3
K [m/s]	Hydraulic conductivity	1.62×10^{-4} – 2.62×10^{-3}
D_m [m ² /s]	Molecular diffusion coefficient	5.0×10^{-9}
θ [1]	Porosity	0.36
D_{50} [mm]	Median grain size	0.264
α_L [m]	Longitudinal dispersivity	0.01
α_T [m]	Transverse dispersivity	0.001
K_O [mg/L]	Half-saturation constant for dissolved oxygen	6.5
c_O [mg/L]	Oxygen concentration in stream	7.36
R_O [umol/ Lh]	Maximum rate of oxygen consumption	41.43–64.76

The hyporheic exchange flux was calculated using NaCl tracer experiment in each flow condition, and the oxygen concentration in sediments was measured with a planar optode system.

The volumetric oxygen consumption rate R_O in experiments was determined by hyporheic exchange flux and oxygen concentration. We used the term R_O as maximum consumption rate of oxygen in our model and adjusted the numerical model parameters for fitting the simulated result to experimental data (Tables S1, S2).

Table S2. Hydraulic conditions of the flume experiments of Wolke et al. (2019)

Run	Set	U	H_d	u_c	H	R_O
1	1	0.16	1.50	0	14.2	64.76
	2	0.16	1.94	0	14.2	61.43
2	1	0.25	1.13	0.035	13.8	43.33
	2	0.25	1.13	0.049	13.7	57.62
3	1	0.28	1.37	0.14	14.2	52.38
	2	0.29	1.37	0.135	13.9	49.05
4	1	0.32	1.38	0.394	14.2	53.33
	2	0.32	1.38	0.275	14.2	42.86
5	1	0.36	1.41	0.699	14.3	41.43
	2	0.37	1.41	0.644	13.8	21.90

Text 2. Simulation scenarios

Table S3. Parameters for bedform properties and hydraulic conditions used in this study

D_{50}	Re	U	D^*	T	S	τ_{cr}^*	u^*	τ^*	u_{cr}^*	u_c
[mm]		[m/s]					[m/s]			
0.08	2000	0.100	2.037	-0.269	8.62E-5	0.089	0.0093	0.065	0.011	0
	2500	0.125	2.037	0.142	1.35E-4	0.089	0.0116	0.102	0.011	0.11
	3000	0.150	2.037	0.645	1.94E-4	0.089	0.0139	0.147	0.011	1.98
	3500	0.175	2.037	1.239	2.64E-4	0.089	0.0162	0.200	0.011	6.67
	4000	0.200	2.037	1.924	3.45E-4	0.089	0.0186	0.261	0.011	14.83
	4500	0.225	2.037	2.701	4.36E-4	0.089	0.0209	0.331	0.011	27.08
0.15	2500	0.125	3.819	-0.058	1.35E-4	0.058	0.0116	0.054	0.012	0
	3000	0.150	3.819	0.356	1.94E-4	0.058	0.0139	0.078	0.012	1.04

D_{50}	Re	U	D^*	T	S	τ_{cr}^*	u^*	τ^*	u_{cr}^*	u_c
[mm]		[m/s]					[m/s]		[m/s]	
	3500	0.175	3.819	0.845	2.64E-4	0.058	0.0162	0.107	0.012	5.39
	4000	0.200	3.819	1.410	3.45E-4	0.058	0.0186	0.139	0.012	13.87
	4500	0.225	3.819	2.051	4.36E-4	0.058	0.0209	0.176	0.012	27.25
	5000	0.250	3.819	2.766	5.39E-4	0.058	0.0232	0.218	0.012	46.32
0.22	2500	0.125	5.601	-0.170	1.35E-4	0.045	0.0116	0.037	0.013	0
	3000	0.150	5.601	0.195	1.94E-4	0.045	0.0139	0.053	0.013	0.45
	3500	0.175	5.601	0.627	2.64E-4	0.045	0.0162	0.073	0.013	4.24
	4000	0.200	5.601	1.125	3.45E-4	0.045	0.0186	0.095	0.013	12.63
	4500	0.225	5.601	1.690	4.36E-4	0.045	0.0209	0.120	0.013	26.52
	5000	0.250	5.601	2.321	5.39E-4	0.045	0.0232	0.148	0.013	46.79
0.36	3000	0.150	9.165	-0.046	1.94E-4	0.034	0.0139	0.033	0.014	0
	3500	0.175	9.165	0.299	2.64E-4	0.034	0.0162	0.044	0.014	1.72
	4000	0.200	9.165	0.696	3.45E-4	0.034	0.0186	0.058	0.014	8.68
	4500	0.225	9.165	1.147	4.36E-4	0.034	0.0209	0.073	0.014	21.99
	5000	0.250	9.165	1.650	5.39E-4	0.034	0.0232	0.091	0.014	42.72
	5500	0.275	9.165	2.207	6.52E-4	0.034	0.0255	0.110	0.014	71.93
	6000	0.300	9.165	2.816	7.76E-4	0.034	0.0278	0.131	0.014	110.70