Sensitivity analysis

This document lists the biogeochemical constants used in the model together with their sensitivities. The sensitivities are calculated in the following way: For each parameter, two perturbed runs of the model were performed for each of the seven stations, with the parameter value increased or decreased by 1%. The score which measures the model fit to the observed pore water concentrations is then calculated as described in the article. We define the sensitivity as the relative change of the model score divided by the relative change in the parameter. That is, a change of the model score by 1% yields a sensitivity of 1.0 in our case. The average value between increased and decreased experiment is given for each of the parameters.

There are two classes of parameters.

- The first ones are global parameters with the same value at all stations. These are given in the table on the next two pages.
- The second ones are local parameters valid at individual stations only. These are given on the last page.

constant	value	sensitivity	description
r_max_lib_mn2_pyrox	1e-05	1.696	maximum rate of mn2 liberation due to pyrite reduction [mol/kg/d]
mos_min_sed_irred	4e-04	1.462	iron hydroxide half-saturation concentration for detritus remineralization by iron reduction [mol/kg]
r_max_ox_pyr	0.1	1.084	maximum oxidation rate of pyrite [1/d]
so4_min_det_sulf	1e-06	0.795	minimum sulfate concentration for sulfate reduction [mol/kg]
ihs_min_sed_irred	0.0065	0.745	iron hydroxide half-saturation concentration for detritus remineralization by iron reduction [mol/kg]
p_content_im	2e-04	0.735	mass fraction of phosphate that can be adsorbed/desorbed to illite-montmorillonite mixed layer minerals [1]
k_mno2_h2s	58.4	0.685	rate constant for manganese oxide reduction by h2s [kg/mol/d]
k_pyrite	8.9	0.657	rate constant for formation of pyrite [kg/mol/d]
r_h3o_ads	0.1	0.610	rate of proton adsorption to illite-montmorillonite mixed layer minerals [1/d]
k_nh4_o2	274000	0.605	nitrification rate for ammonium in the sediment at 0 deg C [1/d]
k_h2s_no3	438	0.599	reaction constant h2s oxidation with no3 [kg/mol/day]
o2_min_nit	1e-06	0.588	oxygen half-saturation constant for nitrification [mol/kg]
k_o2_pyr	1.93	0.585	rate coefficient for oxygen consumption by pyrite oxidation [kg/mol/d]
k_mno2_fe2	5.48	0.520	rate constant for MnO2 reduction by Fe2+ [kg/mol/d]
k_sul_o2	20000	0.506	reaction constant sul oxidation with o2 [kg/mol/day]
r_ims_diss	0.001	0.480	rate of iron monosulfide dissolution [1/d]
k_ims_o2	1062	0.479	rate constant for ims oxidation by O2 [kg/mol/d]
r_po4_ads_pim	0.1	0.418	rate of phosphate adsorption/desorption to illite-montmorillonite [1/d]
r_iim_diss	0.001	0.406	dissilution rate of iron adsorbed to illite-montmorillonite mixed-layer minerals [1/d]
k_sul_no3	20000	0.390	reaction constant sul oxidation with no3 [kg/mol/day]
o2_min_sed_resp	2e-05	0.370	oxygen half-saturation constant for recycling of sediment detritus using oxygen [mol/kg]
po4_ads_pim	3e-05	0.287	phosphate concentration when phosphate in illite-montmorillonite mixed layer minerals is fully adsorbed [mol/kg]

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constant	value	sensitivity	description
fe_content_im	0.001	0.274	potentially reducible iron content of illite-montmorillonite mixed layer minerals [g/g]
k_h2s_o2	438	0.273	reaction constant h2s oxidation with o2 [kg/mol/day]
k_h2s_ihs	21.9	0.226	rate constant for hydrogen sulfide oxidation in presence of iron-III minerals [1/d]
r_i2i_ox	0.1	0.192	rate of oxidation of iron-II in illite-montmorillonite mixed-layer minerals [1/d]
factor_pref_remin_p	10	0.177	acceleration factor for preferential mineralization of P compared to N under hypoxic conditions [1]
r_h2s_ox_i3i	0.1	0.174	rate of h2s reduction by i3i oxidation [1/d]
r_max_lib_mn2_pyrox	1e-05	1.696	maximum rate of mn2 liberation due to pyrite reduction [mol/kg/d]
k_mno2	548000	0.172	oxidation constant for manganese-II [kg3/mol3/d]
k_ips_dissolution	0.1	0.167	inverse timescale for dissolution of iron phosphate [1/d]
no3_min_sed_denit	4e-06	0.076	nitrate half-saturation concentration for denitrification in the water column [mol/kg]
vel_remin_deep	3.556e-11	0.065	effective velocity of detritus mineralization in the deepest layer [m/s]
r_ihs_trans_ihc	0.00164	0.028	transformation rate from amorphous to crystalline iron hydroxide [1/d]
ks_fes	0.00631	0.000	saturation constant for iron monosulfide solubility [mol/kg]

constant	station	value	sensitivity	description
r_fluffy_moveaway	LB	0	-	rate with which
	MB	0	-	fluffy layer is
	ST	0.22	0.120	transported to
	DS	0.298	0.020	deeper areas [1/d]
	AB	0	-	
	TW	0.005	0.413	
	OB	0.22	0.067	
accratedet	LB	5.6	0.520	accumulation ratio
	MB	3	0.043	of detritus
	ST	0	-	(import vs.
	DS	4	0.024	local production) [1]
	AB	3	0.289	
	TW	0	-	
	OB	8	0.018	
ratio_Mn_Fe	LB	0.02	0.346	ratio between
	MB	0.04	0.046	manganese oxides and
	ST	0.04	0.083	iron oxyhydroxides
	DS	0.04	0.027	that are imported/
	AB	0.01	0.264	precipitate in the
	TW	0.028	0.383	water column
	OB	0.076	0.011	
vol_fraction_im	LB	0.5	0.604	fraction of
	MB	0.5	0.312	illite-montmorillonite
	ST	0.007	0.113	mixed layer minerals
	DS	0.088	0.035	on volume of
	AB	0.5	0.216	all minerals [1]
	TW	0.5	0.302	
	OB	0.01	0.010	
ihs_deposition	LB	0.35	0.512	ratio between
	MB	1.4	0.073	iron hydroxide
	ST	0.7	0.000	and local
	DS	0.7	0.031	detritus deposition [1]
	AB	0.7	0.380	
	TW	0.7	0.000	
	OB	1.33	0.007	
ihs_deposition_moveaway	LB	0	-	value for vertical
	MB	0	-	ihw flux to sediment
	ST	0.0026	0.029	that compensates for
	DS	0.002	0.037	transport to
	AB	0.002	0.000	deeper basins [1]
	TW	0.05	0.147	
	OB	0.0032	0.011	