The following supplement accompanies the article

Modelling sediment assimilative capacity and organic carbon degradation efficiency at marine fish farms

Francisco Bravo*, Jonathan Grant

*Corresponding author: bravofco@gmail.com

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Table S1: Model equations summary. Production-consumption rates of solid and dissolved compounds in µmol cm^{-3} solid d^{-1} and in µmol cm^{-3} porewater d^{-1}, respectively. POC: particulate organic carbon; OR: oxygen reduction (or oxic respiration); SR: sulfate reduction; IR: iron reduction; RO: re-oxidation; φ_S: solid porosity $(1-\varphi)$; *M*: microbial activity; R: reaction. See Table S2 for reaction terms (R1–R9) and Table S6 for model parameters.

Reaction	**Eq.**
$\sum R(\mathrm{POC}) = -(\mathrm{R2a} + \mathrm{R3a} + \mathrm{R4a})$	S1
$\sum R(\mathrm{Waste}) = -(\mathrm{R2b} + \mathrm{R3b} + \mathrm{R4b})$	S2
$\sum R(\mathrm{O_2}) = \frac{\varphi_S}{\varphi} * \mathrm{R2} * \gamma\mathrm{OR}_{\mathrm{O_2}}^{\mathrm{POC}} - \mathrm{R5} * \gamma\mathrm{RO}_{\mathrm{O_2}}^{\mathrm{Total\ S^{2-}}} - \mathrm{R6}$	S3
$\sum R(\mathrm{SO_4}) = \mathrm{R5} - \frac{\varphi_S}{\varphi} * \mathrm{R3} * \gamma\mathrm{SR}_{\mathrm{SO_4^{2-}}}^{\mathrm{POC}}$	S4
$\sum R(\mathrm{FeOOH}) = \frac{\varphi}{\varphi_S} * \mathrm{R6} * \gamma\mathrm{RO}_{\mathrm{O_2}}^{\mathrm{Fe^{2+}}} - \mathrm{R4} * \gamma\mathrm{IR}_{\mathrm{FeOOH}}^{\mathrm{POC}} - \mathrm{R7}$	S5
$\sum R(\mathrm{Total\ S^{2-}}) = \frac{\varphi_S}{\varphi} * \left(\mathrm{R3} * \gamma\mathrm{SR}_{\mathrm{SO_4^{2-}}}^{\mathrm{POC}} - \mathrm{R7} * \gamma\mathrm{RO}_{\mathrm{FeOOH}}^{\mathrm{H_2S}} - \mathrm{R8}\right) - \mathrm{R5}$	S6
$\sum R(\mathrm{Fe^{2+}}) = \frac{\varphi_S}{\varphi} * (\mathrm{R4a} + \mathrm{R4b}) * \gamma\mathrm{IR}_{\mathrm{FeOOH}}^{\mathrm{POC}} + \frac{\varphi_S}{\varphi} * (\mathrm{R7} - \mathrm{R8}) - \mathrm{R6} * \gamma\mathrm{RO}_{\mathrm{O_2}}^{\mathrm{Fe^{2+}}}$	S7
$\sum R(\mathrm{FeS}) = \mathrm{R8} - \mathrm{R9}$	S8
$\sum R(\mathrm{M}) = \alpha_M(\mathrm{R2} + \mathrm{R3} + \mathrm{R4}) * M * \left(1 - \frac{M}{\lambda_M * ([\mathrm{POC_{SL}}] + [\mathrm{Waste_{SL}}])}\right)$	S9

Table S2: Mathematical expression of redox reactions R1 to R9 (Table 2). R1 in µmol cm^{-2}d^{-1} and R2 to R9 in µmol cm^{-3}d^{-1}. POC: particulate organic carbon; OR: oxygen reduction (or oxic respiration); SR: sulfate reduction; IR: iron reduction; *M*: microbial activity; SL: sediment layer; WC: water column; R: reaction. See Table S5 for partitioning factors (PF) and Table S6 for model parameters

Water column – Partially stratified layer (WC)		
(R1)	POC consumption by oxic respiration	$\mathrm{R_{OR,WC}} * [\mathrm{POC_{WC}}]$
Sediment – Oxic/Anoxic layer (SL)		
(R2a)	POC consumption by O_2 reduction	$\mathrm{R_{OR,SL}} * [\mathrm{POC}] * [M] * \mathrm{PF}_{M,\mathrm{OR}}$
(R3a)	POC consumption by SO_4^{2-} reduction	$\mathrm{R_{SR,SL}} * [\mathrm{POC}] * [M] * \mathrm{PF}_{M,\mathrm{SR}}$
(R4a)	POC consumption by Fe^{3+} reduction	$\mathrm{R_{IR,SL}} * [\mathrm{POC}] * [M] * \mathrm{PF}_{M,\mathrm{IR}}$
(R2b)	Organic waste consumption by O_2 reduction	$\mathrm{R_{OR,SL}} * [\mathrm{Waste}] * [M] * \mathrm{PF}_{M,\mathrm{OR}}$
(R3b)	Organic waste consumption by SO_4^{2-} reduction	$\mathrm{R_{SR,SL}} * [\mathrm{Waste}] * [M] * \mathrm{PF}_{M,\mathrm{SR}}$
(R4b)	Organic waste consumption by Fe^{3+} reduction	$\mathrm{R_{IR,SL}} * [\mathrm{Waste}] * [M] * \mathrm{PF}_{M,\mathrm{IR}}$
(R5)	SO_4^{2-} production by Total S^{2-} reoxidation with O_2	$k_{\mathrm{Total\ S^{2-}_{SL,ox1}}} * [\mathrm{Total\ S^{2-}}] * [\mathrm{O_2}]$
(R6)	Fe^{2+} reoxidation with O_2	$k_{\mathrm{Fe,ox}} * [\mathrm{Fe^{2+}}] * [\mathrm{O_2}]$
(R7)	Total S^{2-} reoxidation with iron oxides	$k_{\mathrm{Total\ S^{2-}_{SL,ox2}}} * [\mathrm{Total\ S^{2-}}] * [\mathrm{Fe^{2+}}]$
(R8)	Total S^{2-} precipitation to FeS	$k_{\mathrm{FeSppt}} * ([\mathrm{Fe^{2+}}] * [\mathrm{Total\ S^{2-}}] - K_{\mathrm{sp}}\mathrm{FeS})$
(R9)	FeS precipitation to FeS_2	$k_{\mathrm{FeS_2}} * [\mathrm{FeS}]$

Table S3: Transport processes in bottom water. WC: water column; BC: bottom water; u_{WC}: free-stream bottom current speed (see Table S6)

Bottom water (WC)		
(T1)	Bottom water O_2 renewal	$u_{WC} * ([O_{2,WC,BC}] - [O_{2,WC}])$
(T2)	Bottom water SO_4^{2-} renewal	$u_{WC} * ([SO_{4,WC,BC}^{2-}] - [[SO_{4,WC}^{2-}])$
(T3)	Bottom water Total S^{2-} renewal	$u_{WC} * ([Total\, S_{WC,BC}^{2-}] - [Total\, S_{WC}^{2-}])$

Table S4: Kinetic terms of reactions R1 to R9 (Table 2, Table S2). Note that all reactions are adjusted by a dimensionless temperature factor. See Table S6 for model parameters. $\mathrm{R_{OR,WC}}$: specific rate of oxic respiration in the water column; $\mathrm{R_{OR,SL}}$: specific rate of oxic respiration in the sediment; $\mathrm{R_{SR,SL}}$: specific rate of sulfate reduction in the sediment; $\mathrm{R_{IR,SL}}$: specific rate of iron respiration in the sediment. All in unit of d^{-1}.

Kinetic terms
$\mathrm{R_{OR,WC}} = \mathrm{R_{OR,WC}^{max}} * \left([\mathrm{O_2}] - [\mathrm{O_{2,min}}]\right)$
$\mathrm{R_{OR,SL}} = \mathrm{R_{OR,SL}^{max}} * \frac{[\mathrm{O_2}]}{K_{\mathrm{s,OR}} + [\mathrm{O_2}]}$
$\mathrm{R_{SR,SL}} = \mathrm{R_{SR,SL}^{max}} * \frac{[\mathrm{SO_4^{2-}}]}{K_{\mathrm{s,SR}} + [\mathrm{SO_4^{2-}}]} * \frac{K_{\mathrm{in,SR}}}{K_{\mathrm{in,SR}} + [\mathrm{O_2}]}$
$\mathrm{R_{IR,SL}} = \mathrm{R_{IR,SL}^{max}} * \frac{[\mathrm{FeOOH}]}{K_{\mathrm{s,IR}} + [\mathrm{FeOOH}]} * \frac{K_{\mathrm{in,IR}}}{K_{\mathrm{in,IR}} + [\mathrm{O_2}]}$

Table S5: Forcing functions. See Table S6 for parameter definitions.

Forcing functions	
Free-stream bottom current speed (u_{WC}):	
$u_{\mathrm{WC}} = u_{\mathrm{WC,mean}} * 1.025 * \cos\left(1 + \left(\frac{2\pi * day\ of\ year}{tidal\ period} + \frac{\pi}{2}\right)\right)$	S10
Shear or frictional velocity at the seabed:	
$u_* = u_{\mathrm{WC}} * \frac{\kappa}{\ln\frac{z_{\mathrm{BBL}}}{z_0}}$	S11
Shear stress exerted by u_{WC}:	
$\tau_u = \rho_{\mathrm{SW}} * u_*^2$	S12
Dispersion area (m^2) of organic waste in the water column:	
$D_{\mathrm{Waste}} = Z_{\mathrm{WC}} * \frac{u_{\mathrm{WC,mean}}}{w_{\mathrm{pellet\ and\ feces}}}$	S13
Gross deposition of organic wastes ($\tau_u < \tau_{\mathrm{cd}}$):	
$\mathrm{Waste}_{\mathrm{flux,SWI}} = \mathrm{Waste}_{\mathrm{dep}} * \left(1 - \frac{\tau_{\mathrm{u}}}{\tau_{\mathrm{cd}}}\right)$	S14
Erosion rate of organic wastes ($\tau_u > \tau_{\mathrm{ce}}$):	
$\mathrm{Waste}_{\mathrm{flux,SWI}} = k_{\mathrm{waste}} * \left(\frac{\tau_u}{\tau_{\mathrm{ce}}} - 1\right)$	S15
Attenuation of bio-transport:	
$K_{\mathrm{v}} = 1 - \frac{[\mathrm{Total\ S^{2-}}]}{[\mathrm{Total\ S^{2-}_{ref}}]}$	S16
Partitioning factor of microbial activity:	
$\mathrm{f_{OR}} = \frac{[\mathrm{O_2}]}{K_{\mathrm{s,OR}} + [\mathrm{O_2}]}$	S17
$\mathrm{f_{SR}} = \frac{[\mathrm{SO_4^{2-}}]}{K_{\mathrm{s,SR}} + [\mathrm{SO_4^{2-}}]} * \frac{K_{\mathrm{in,SR}}}{K_{\mathrm{in,SR}} + [\mathrm{O_2}]}$	S18
$\mathrm{f_{IR}} = \frac{[\mathrm{FeOOH_{SL}}]}{K_{\mathrm{s,IR}} + [\mathrm{FeOOH_{SL}}]} * \frac{K_{\mathrm{in,IR}}}{K_{\mathrm{in,IR}} + [\mathrm{O_2}]}$	S19
$\mathrm{PF}_{M,\mathrm{OR}} = \frac{\mathrm{f_{OR}}}{\mathrm{f_{OR}} + \mathrm{f_{SR}} + \mathrm{f_{IR}}}$	S20
$\mathrm{PF}_{M,\mathrm{SR}} = \frac{\mathrm{f_{SR}}}{\mathrm{f_{OR}} + \mathrm{f_{SR}} + \mathrm{f_{IR}}}$	S21
$\mathrm{PF}_{M,\mathrm{IR}} = \frac{\mathrm{f_{IR}}}{\mathrm{f_{OR}} + \mathrm{f_{SR}} + \mathrm{f_{IR}}}$	S22

Table S6: Model parameters. POC: particulate organic carbon; HSC: half saturation constant; OR: oxygen reduction (or oxic respiration); SR: sulfate reduction; IR: iron reduction; SL: sediment layer; WC: water column; BBL: benthic boundary layer, SWI: sediment water interface; HSC: half-saturation constant.

Parameter	Description / Name	Values	Units	References
κ	Von Kárman constant	0.4	dimensionless	(–)
$k_{\mathrm{Total\ S_{SL}^{2-},ox1}}$	Sulfide oxidation reaction velocity with O_2	164.4	$cm^3 \mu mol^{-1} d^{-1}$	Boudreau (1996)
$k_{\mathrm{Total\ S_{SL}^{2-},ox2}}$	Sulpfide oxidation reaction velocity with FeOOH	274.0	$cm^3 \mu mol^{-1} d^{-1}$	Boudreau (1996)
$k_{\mathrm{Fe,ox}}$	Rate constant for Fe^{2+} oxidation by O_2	109.6	$cm^3 \mu mol^{-1} d^{-1}$	Boudreau (1996)
$k_{\mathrm{FeS_2}}$	Rate constant for FeS_2 formation from FeS	2.73E-6	d^{-1}	Boudreau et al. (1998)
k_{FeSppt}	Rate constant for FeS precipitation from Fe^{2+}	0.821	$cm^3 \mu mol^{-1} d^{-1}$	Boudreau et al. (1998)
k_{waste}	Erosion rate coefficient of organic C associated with fish farm wastes	194.2	$\mu mol\ C\ cm^{-2} d^{-1}$	Cromey et al. (2002)
u_{WC}	Free-stream bottom current speed	0 – 23	$cm\ s^{-1}$	Specific for this study
w_{s}	Settling velocity of suspended POC	520	$cm\ d^{-1}$	Alber (2000)
w_{feed}	Sinking speed of feed pellets	10.89	$cm\ s^{-1}$	Stucchi et al. (2005)
w_{feaces}	Sinking speed of feces	3	$cm\ s^{-1}$	Stucchi et al. (2005)
z_{BBL}	Height above the bottom	100	cm	Specific for this study
z_0	Bed roughness length	0.013-0.1	cm	Soulsby (1997)
Z_{WC}	Water column depth below the fish cage	20	m	Specific for this study
$D_{\mathrm{Total\ S^{2-}}}$	Diffusion coefficient of dissolved sulfide in sediment at 14 °C	0.78	$cm^2 d^{-1}$	Fossing et al. (2004)
$D_{\mathrm{Fe^{2+}}}$	Diffusion coefficient of iron in sediment at 14 °C	0.32	$cm^2 d^{-1}$	Fossing et al. (2004)
$D_{\mathrm{O_2}}$	Diffusion coefficient of oxygen in sediment at 14 °C	1.04	$cm^2 d^{-1}$	Fossing et al. (2004)
$D_{\mathrm{SO_4}}$	Diffusion coefficient of sulfate in sediment at 14 °C	0.48	$cm^2 d^{-1}$	Fossing et al. (2004)
D_{b}	Biodiffusion coefficient	0.15	$cm^2 d^{-1}$	Middelburg et al. (1997)
$\mathrm{FeOOH_{dep}}$	FeOOH deposition rate	0.0175	$\mu mol\ cm^{-2} d^{-1}$	Fossing et al. (2004)
$K_{\mathrm{s,OR}}$	HSC for O_2 limitation in OR	0.004	$\mu mol\ cm^{-3}$	Pastor et al. (2011)
$K_{\mathrm{s,SR}}$	HSC for SO_4^{2-} limitation in SR	1.6	$\mu mol\ cm^{-3}$	Shafei (2012)
$K_{\mathrm{s,IR}}$	HSC for FeOOH limitation in SR	2.45	$\mu mol\ cm_{solid}^{-3}$	Specific for this study
$K_{\mathrm{in,SR}}$	HSC for O_2 inhibition in SR	0.01	$\mu mol\ cm^{-3}$	Specific for this study
$K_{\mathrm{in,IR}}$	HSC for O_2 inhibition in IR	0.01	$\mu mol\ cm^{-3}$	Soetaert et al. (1996)
$K_{\mathrm{sp}}\mathrm{FeS}$	Solubility product constant of FeS	0.0523	$(\mu mol\ cm^{-3})^2$	Boudreau (1996)
$\mathrm{POC_{flux,SWI}}$	Natural POC deposition rate	2	$\mu mol\ C\ cm^{-2} d^{-1}$	Specific for this study
$R_{\mathrm{OR,WC}}^{\mathrm{max}}$	The aerobic decomposition coefficient in the water column	0.00524	$cm^4 \mu mol^{-1} d^{-1}$	Omori et al. (1994)
$R_{\mathrm{POC,SL}}^{\mathrm{max}}$	Maximum oxidation rate of POC	2.73E-4	d^{-1}	Brigolin et al. (2009)
$R_{\mathrm{Waste,SL}}^{\mathrm{max}}$	Maximum oxidation rate of organic waste	0.0027	d^{-1}	Brigolin et al. (2009)
τ_{ce}	Critical shear stress for resuspension of POC and fish farm wastes	0.0179	$N\ m^{-2}$	Cromey et al. (2002)
τ_{cd}	Critical shear stress for deposition of POC and fish farm wastes	0.004	$N\ m^{-2}$	Cromey et al. (2002)
$[O_{2,\mathrm{min}}]$	Limiting O_2 concentration for oxic mineralization in the water column	0.0625	$\mu mol\ cm^{-3}$	Specific for this study.
$[\mathrm{Total\ S_{ref}^{2-}}]$	Toxic H_2S concentration for macrofauna	5	$\mu mol\ cm^{-3}$	Brigolin et al. (2009)
α_M	Transformation rate of POC into microbial activity (*M*)	0.3	$cm^3\ (\mu mol\ C)^{-1}$	Talin et al. (2003)
w_{sed}	Burial velocity of POC and solids	7.123E-4	$cm\ d^{-1}$	Omori et al. (1994)
λ_M	Microbial activity (*M*) to POC ratio	2.52E-4	$cm^3\ (\mu mol\ C)^{-1}$	Talin et al. (2003)
$\gamma \mathrm{OR_{O_2}^{POC}}$	Mole O_2 reduced per mole of POC oxidized	1.3	$mol\ O_2\ (mol\ C)^{-1}$	Pastor et al. (2011), Soetaert et al. (1996)
$\gamma \mathrm{RO_{O_2}^{Total\ S^{2-}}}$	Mole of O_2 reduced per mole of Total S^{2-} oxidized	2	$mol\ O_2\ (mol\ Total\ S^{2-})^{-1}$	Pastor et al. (2011), Soetaert et al. (1996)
$\gamma \mathrm{RO_{O_2}^{Fe^{2+}}}$	Mole of Fe^{2+} oxidized per mole of O_2 reduced	4	$mol\ Fe^{2+}\ (mol\ O_2)^{-1}$	Pastor et al. (2011), Soetaert et al. (1996)
$\gamma \mathrm{SR_{SO_4^{2-}}^{POC}}$	Mole of SO_4^{2-} reduced per mole of POC oxidized	0.5	$mol\ SO_4^{2-}\ (mol\ C)^{-1}$	Pastor et al. (2011), Soetaert et al. (1996)
$\gamma \mathrm{IR_{Fe^{2+}}^{POC}}$	Mole of FeOOH reduced per mole of POC oxidized	4	$mol\ Fe^{2+}\ (mol\ C)^{-1}$	Specific for this study
$\gamma \mathrm{RO_{FeOOH}^{H_2S}}$	Mole of Total S^{2-} oxidized per mole of FeOOH reduced to particulate S (S^0)	0.5	$mol\ Total\ S^{2-}\ (mol\ FeOOH)^{-1}$	Specific for this study
φ	Sediment porosity	0.8	dimensionless	Specific for this study
ρ	Sediment density	2.45	$g\ cm^{-3}$	Specific for this study
ρ_{SW}	Seawater density	1.027	$g\ cm^{-3}$	Specific for this study
ν	Exchange velocity of solutes due to bioturbation	3	$cm\ d^{-1}$	Hammond & Fuller (1979)

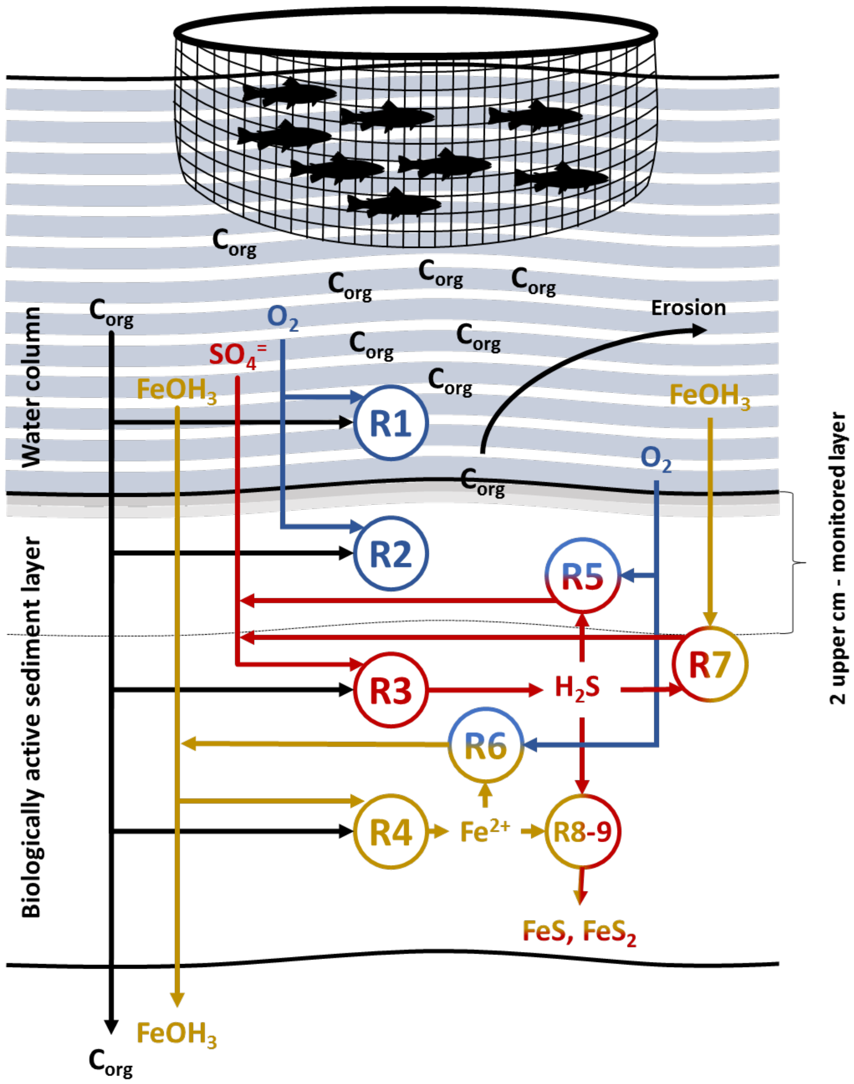

Figure S1: Conceptual model representation. See Table 2 in the main article and Table S2 for redox reactions (R1–R9). C_{org}: organic carbon

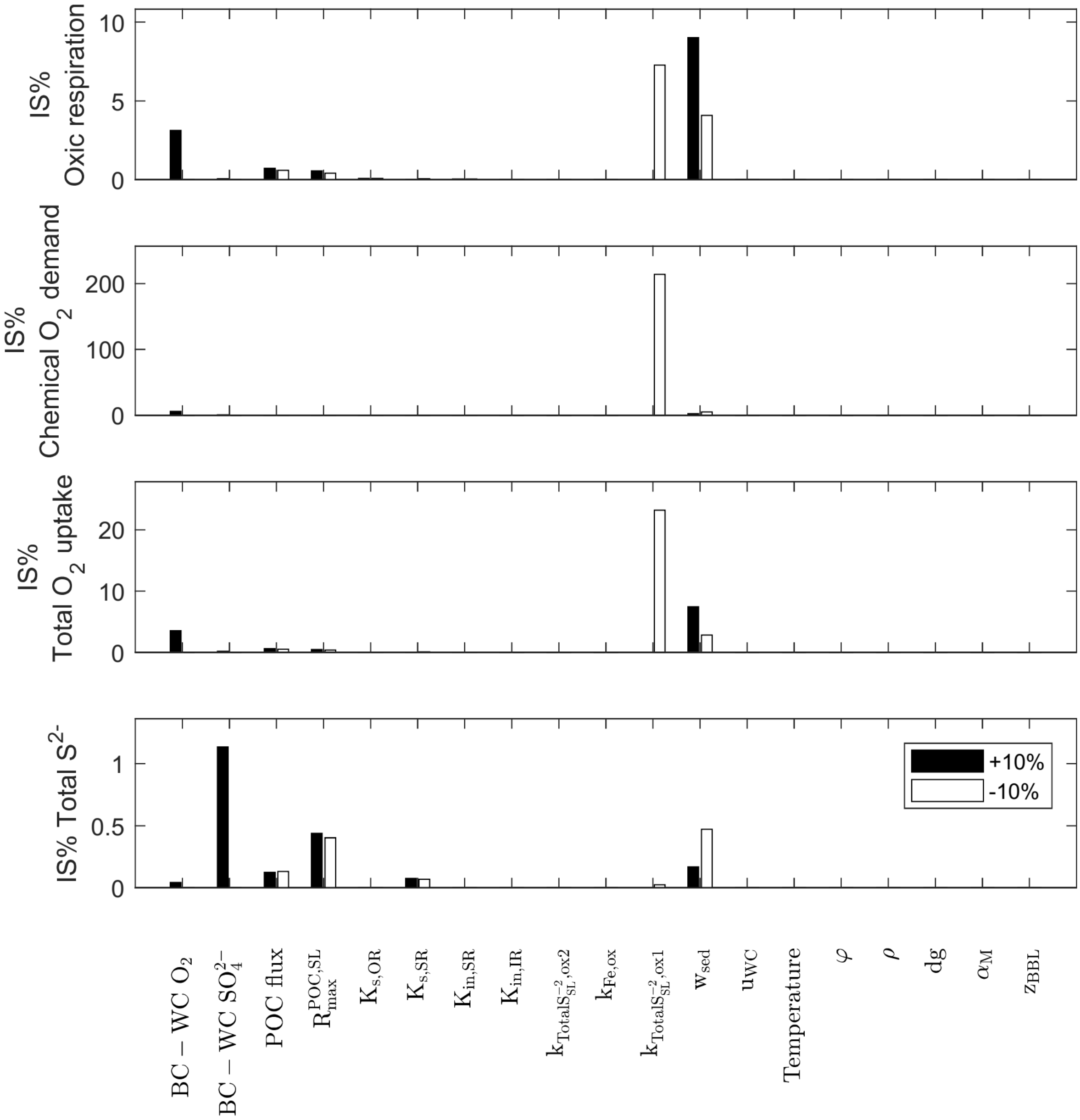

Figure S2: Sensitivity of state variables to +/- 10% changes in model parameters. Positive sensitivity index (IS%) values mean that changes in model parameter increase state variable, and vice versa. Increase in state variable is observed. Parameters and specific ranges used in sensitivity are specified in Table S7.

Table S7. Model parameters tested for sensitivity. Ranges of variation of model parameters were defined from literature and natural ranges of oscillation in coastal waters (solute concentrations and particulate organic carbon (POC) deposition).

Parameter	Min	Max	Range	Units	Description
$O_{2,BC-WC}$	0	300	300	µmol cm^{-3}	Far field O_2 in water column
$SO_{4,BC,WC}$	0	28	28	µmol cm^{-3}	Far field O_2 in water column
POC flux	0	13.68	13.68	µmol cm^{-2} d^{-1}	Ambient POC deposition
$R_{\mathrm{POC,SL}}^{\mathrm{max}}$	2.74E-06	0.0002	0.0003	d^{-1}	Maximum oxidation rate of POC
$K_{\mathrm{s,OR}}$	1.00E-03	0.01	0.009	µmol cm^{-3}	HSC for O_2 limitation in oxic respiration.
$K_{\mathrm{s,SR}}$	0.05	1.6	1.55	µmol cm^{-3}	HSC for SO_4 limitation in SR.
$K_{\mathrm{in,SR}}$	1.00E-03	0.01	0.009	µmol cm^{-3}	HSC for O_2 inhibition of SR
$K_{\mathrm{in,IR}}$	1.00E-03	0.01	0.009	µmol cm^{-3}	HSC for O_2 inhibition of IR
$k_{\mathrm{Total\ S_{SL}^{-2},ox2}}$	2.74E-02	273.79	273.76	cm^3 µmol^{-1} d^{-1}	Rate constant for sulfide oxidation by FeOOH
$k_{\mathrm{Fe,ox}}$	273.90	2739.70	2465.8	cm^3 µmol^{-1} d^{-1}	Rate constant for Fe^{2+} oxidation by O_2
$k_{\mathrm{Total\ S_{SL}^{-2},ox1}}$	0.8767	4380	4382.72	cm^3 µmol^{-1} d^{-1}	Rate constant for sulfide oxidation by O_2
w_{sed}	0.0002	0.0275	0.0271	cm d^{-1}	Burial velocity at the sediment-water interface
u_{WC}	259200	950400	691200	cm d^{-1}	Free-stream bottom current speed
Temperature	5	15	10	°C	Temperature
φ	0.5	0.9	0.4	dimensionless	Sediment porosity
ρ	1.5	2.5	1	g of sediment cm^{-3} of dry sediment	Sediment density
dg	0.044	0.35	0.306	mm	Grain size diameter
α_M	0.2	0.4	0.2	cm^3 (µmol C)$^{-1}$	Transformation rate of POC into microbial activity
z_{BBL}	50	100	50	cm	Height of BBL

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