



Supplement of

FESDIA (v1.0): exploring temporal variations of sediment biogeochemistry under the influence of flood events using numerical modelling

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SUPPLEMENTARY TEXT

Table S1: Full Parameters used in the model

Model Parameters	Model Notation	Values	units	description	References
\overline{flux}_{org}	$CFlux$	150	$mmol\ m^{-2}d^{-1}$	total organic C deposition	Pastor et al 2011
$pfast$	pFast	0.5	-	part FDET in carbon flux	Pastor et al 2011
\overline{flux}_{FeO03}	FeOH3flux	0.01	$mmol\ m^{-2}d^{-1}$	deposition rate of FeOH3	Assumed
rFast	rFast	0.1	d^{-1}	decay rate FDET	Ait Ballagh et al., 2021
rSlow	rSlow	0.0031	d^{-1}	decay rate SDET	Ait Ballagh et al., 2021
NCrFdet	NCrFdet	0.14	$molN/molC$	NC ratio FDET	Pastor et al., 2011
NCrSdet	NCrSdet	0.1	$molN/molC$	NC ratio SDET	Pastor et al., 2011
BCupLiq	BCupLiq	2	-	upper boundary liq. 1:flux, 2:conc, 3:0-grad	
BCdownLiq	BCdownLiq	3	-	lower boundary liq. 1:flux, 2:conc, 3:0-grad	
O_{2bw}	O2bw	197	$mmol\ m^{-3}$	upper boundary O2	Ait Ballagh et al., 2021
NO_{3bw}	NO3bw	0.0	$mmol\ m^{-3}$	upper boundary NO3	Ait Ballagh et al., 2021
NH_{3bw}	NH3bw	0.0	$mmol\ m^{-3}$	upper boundary NH3	Ait Ballagh et al., 2021
CH_{4bw}	CH4bw	0.0	$mmol\ m^{-3}$	upper boundary CH4	Rasmann et al., 2016
DIC	DICbw	2360	$mmol\ m^{-3}$	upper boundary DIC	Pastor et al., 2018
Fe^{2+}_{bw}	Febw	0.0	$mmol\ m^{-3}$	upper boundary Fe2	Pastor et al., 2018
H_2S_{bw}	H2Sbw	0.0	$mmol\ m^{-3}$	upper boundary H2S	Pastor et al., 2018
SO_{4bw}	SO4bw	30246	$mmol\ m^{-3}$	upper boundary SO4	Pastor et al., 2018
w	w	0.027	$cm\ d^{-1}$	advection rate	Pastor et al., 2011
D_0	biot	0.01	$cm^2\ d^{-1}$	bioturbation coefficient	Ait Ballagh et al., 2021
Z_L	biotdepth	5	cm	depth of mixed layer	Ait Ballagh et al., 2021
$biot_{att}$	biotatt	1.0	cm^{-1}	attenuation coeff below biotdepth	Ait Ballagh et al., 2021
Irr_0	irr	0.2	d^{-1}	bio-irrigation rate	Ait Ballagh et al., 2021
Z_{irr}	irrdepth	7	cm	depth of irrigated layer	Ait Ballagh et al., 2021
Irr_{att}	irratt	1.0	cm	attenuation coeff below irrdepth	Ait Ballagh et al., 2021

Model Parameters	Model Notation	Values	units	description	References
$temp$	temperature	16	°C	temperature	Ait Ballagh et al., 2021
sal	salinity	38	psu	salinity	Ait Ballagh et al., 2021
TOC_{ref}	TOC0	1.1	%	refractory Carbon conc	Pastor et al., 2018
ks_{Nitr_i}	ksO2nitori	10	$mmol\ O_2\ m^{-3}$	half-sat O2 in nitrification	Soetaert et al., 1996
ks_{o_2}	ksO2oxic	1.0	$mmol\ O_2\ m^{-3}$	half-sat O2 in oxic mineralisation	Soetaert et al., 1996
ks_{NO_3}	ksNO3denit	10	$mmol\ NO_3\ m^{-3}$	half-sat NO3 in denitrification	Soetaert et al., 1996
k_{inO_2den}	kinO2denit	1.0	$mmol\ O_2\ m^{-3}$	half-sat O2 inhib denitrification	Soetaert et al., 1996
k_{inNO_3ano}	kinNO3anox	10	$mmol\ NO_3\ m^{-3}$	half-sat NO3 inhib anoxic degr	Soetaert et al., 1996
k_{inO_2ano}	kinO2anox	1.0	$mmol\ O_2\ m^{-3}$	half-sat O2 inhib anoxic min	Soetaert et al., 1996
ks_{FeOH_3}	ksFeOH3	12500	$mmol\ FeOH_3$	half-sat FeOH3 conc in iron reduction	Wang and Van Cappellen, 1996
ks_{inFeOH_3ano}	kinFeOH3	12500	$mmol\ FeOH_3$	half-sat FeOH3 inhibition S reduction	Wang and Van Cappellen, 1996
ks_{SO_4}	ksSO4BSR	800	$mmol\ S\ m^{-3}$	half-sat SO4 conc in sulphate reduction	Wang and Van Cappellen, 1996
k_{inSO_4ano}	kinSO4Met	1000	$mmol\ S\ m^{-3}$	half-sat SO4 inhibition methanogenesis	Wang and Van Cappellen, 1996
R_{FeOH_3}	rFeox	0.3	$(mmol\ m^{-3})^-$	Max rate Fe oxidation	Berg et al. 2003
R_{H_2S}	rH2Sox	5×10^{-5}	$(mmol\ m^{-3})^-$	Max rate H2S oxidation	Assumed
$R_{FeSprod}$	rFeS	1×10^{-3}	$(mmol\ m^{-3})^-$	maximum rate FeS production	Assumed
R_{CH_4}	rCH4ox	27	$(mmol\ m^{-3})^-$	Max rate CH4 oxidation with O2	Berg et al. 2003
R_{AOM}	rAOM	3×10^{-5}	$(mmol\ m^{-3})^-$	Max rate anaerobic oxidation Methane	Assumed
\emptyset_0	por0	0.8	-	surface porosity	Ait Ballagh et al., 2021
\emptyset_∞	pordeep	0.6	-	deep porosity	Ait Ballagh et al., 2021

Model Parameters	Model Notation	Values	units	description	References
δ	porcoeff	2	cm	porosity decay coefficient	Ait Ballagh et al., 2021
F	formationtype	1.0	-	formationfactor, 1=sand,2=fine sand,3=general	Pastor et al., 2011
k_{ads}	Kads	1.3	-	Adsoption coefficient	Soetaert et al., 1996a

Table S2: Estimate of relaxation timescale (days) with uncertainty in estimate derived from non-parametric bootstrapping

	O ₂	SO ₄ ²⁻	DIC
EM1 Scenario			
	5 ± 3	117 ± 6	142 ± 23
EM2 Scenario			
	2 ± 2	91 ± 6	103 ± 9

A2 Model Grid

As explained in the main text, the event routine was modified the model grid at the specific time during its runtime. A certain depth of deposition Z_{pert} result to N_{pert} layer added to the model grid N . Afterward, regridding of this layer together with the cell content is performed via interpolation of the grid $N + N_{pert}$ into the model grid. Figure A1 showed the difference in the spacing of the grid Δz and number of layer before and deposition.

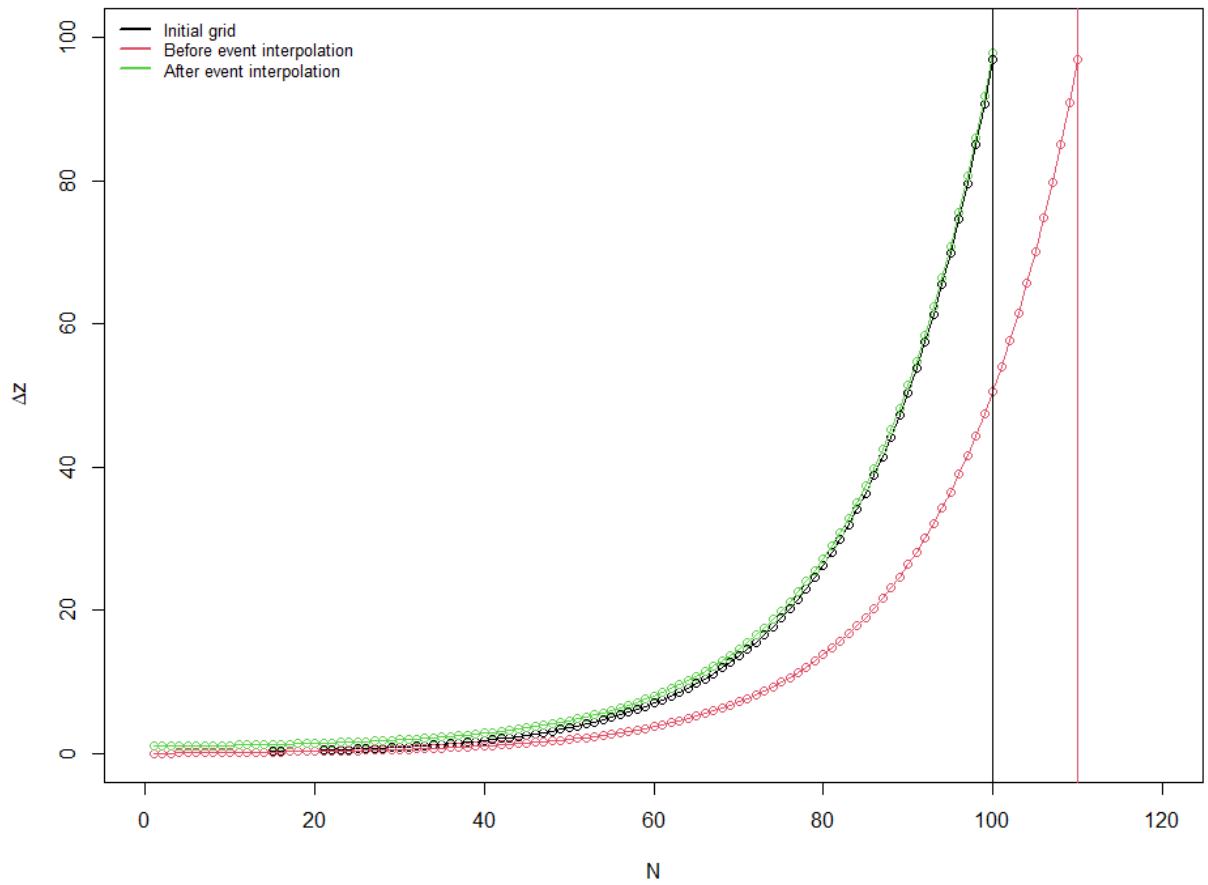


Figure S1: Grid layer in the event routine.