

Electronic Supplementary Material

Benthic-pelagic coupling in the Barents Sea: an integrated data-model framework

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Table S1. Reaction network implemented in the organic matter degradation model for the Barents Sea [1,2].

Reaction	Pathway
<i>Primary redox reactions</i>	
r_1	<i>Aerobic respiration</i>
r_2	<i>Denitrification</i>
r_3	<i>HR Manganese reduction</i>
r_4	<i>HR Iron reduction</i>
r_5	<i>Organoclastic sulfate reduction</i>
r_6	<i>Methanogenesis</i>
<i>Secondary redox reactions</i>	
r_7	<i>Nitrification</i>
r_8	<i>Manganese reoxidation by oxygen</i>
r_9	<i>Iron reoxidation by HR manganese</i>
r_{10}	<i>Iron reoxidation by PR manganese</i>
r_{11}	<i>Iron reoxidation by oxygen</i>
r_{12}	<i>Sulfide oxidation by oxygen</i>
r_{13}	<i>Sulfide oxidation by HR manganese</i>
r_{14}	<i>Sulfide oxidation by PR manganese</i>
r_{15}	<i>Sulfide oxidation by HR iron</i>
r_{16}	<i>Sulfide oxidation by MR iron</i>
r_{17}	<i>Sulfide oxidation by PR iron</i>
r_{18}	<i>Anaerobic oxidation of methane (AOM) coupled to sulfate reduction</i>
r_{19}	<i>Methane oxidation by oxygen</i>
r_{20}	<i>Iron sulfide oxidation by oxygen</i>
<i>Other reactions</i>	
r_{21}	<i>HR Mn ageing</i>
r_{22}	<i>HR Fe ageing</i>

HR (Highly Reactive); MR (Moderately Reactive); (PR) Poorly Reactive

Table S2. Stoichiometry and reaction rates implemented in the organic matter degradation model for the Barents Sea [1,2].

	Stoichiometry	Reaction rate
<i>Primary redox reactions</i>		
r_1	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + (x + 2y)O_2 + (y + 2z)HCO_3^- \rightarrow (x + y + 2z)CO_2 + yNH_4^+ + zHPO_4^{2-} + (x + 2y + 2z)H_2O$	$r_1 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{O_2}$
r_2	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + \left(\frac{4x+3y}{5}\right)NO_3^- \rightarrow \left(\frac{2x+4y}{5}\right)N_2 + \left(\frac{x-3y+10z}{5}\right)CO_2 + \left(\frac{4x+3y-10z}{5}\right)HCO_3^- + zHPO_4^{2-} + \left(\frac{3x+6y+10z}{5}\right)H_2O$	$r_2 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{NO_3}$
r_3	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + 2x HR MnO_2 + (3x + y - 2z)CO_2 + (x + y - 2z)H_2O \rightarrow 2xMn^{2+} + (4x + y - 2z)HCO_3^- + yNH_4^+ + HPO_4^{2-}$	$r_3 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{HR MnO_2}$
r_4	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + 4x HR Fe(OH)_3 + (7x + y - 2z)CO_2 \rightarrow 4xFe^{2+} + (8x + y - 2z)HCO_3^- + yNH_4^+ + zHPO_4^{2-} + (3x - y + 2z)H_2O$	$r_4 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{HR Fe(OH)_3}$
r_5	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + \frac{x}{2}SO_4^{2-} + (y - 2z)CO_2 + (y - 2z)H_2O \rightarrow \frac{x}{2}H_2S + (x + y - 2z)HCO_3^- + yNH_4^+ + zHPO_4^{2-}$	$r_5 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{SO_4^{2-}}$
r_6	$(CH_2O)_x(NH_3)_y(H_3PO_4)_z + (y - 2z)H_2O \rightarrow \left(\frac{x-2y+4z}{2}\right)CO_2 + (y - 2z)HCO_3^- + yNH_4^+ + zHPO_4^{2-} + \frac{x}{2}CH_4$	$r_6 = v \cdot (a + age)^{-1} \cdot CH_2O \cdot f_{CH_4}$
<i>Secondary redox reactions</i>		
r_7	$NH_4^+ + 2O_2 + 2HCO_3^- \rightarrow NO_3^- + 2CO_2 + 3H_2O$	$r_7 = k_7 \cdot NH_4^+ \cdot O_2$
r_8	$Mn^{2+} + \frac{1}{2}O_2 + 2HCO_3^- \rightarrow HR MnO_2 + 2CO_2 + H_2O$	$r_8 = k_8 \cdot Mn^{2+} \cdot O_2$
r_9	$2Fe^{2+} + HR MnO_2 + 2HCO_3^- + 2H_2O \rightarrow 2 HR Fe(OH)_3 + Mn^{2+} + 2CO_2$	$r_9 = k_9 \cdot Fe^{2+} \cdot HR MnO_2$
r_{10}	$2Fe^{2+} + PR MnO_2 + 2HCO_3^- + 2H_2O \rightarrow 2 HR Fe(OH)_3 + Mn^{2+} + 2CO_2$	$r_{10} = k_{10} \cdot Fe^{2+} \cdot PR MnO_2$
r_{11}	$Fe^{2+} + \frac{1}{4}O_2 + 2HCO_3^- + \frac{1}{2}H_2O \rightarrow HR Fe(OH)_3 + 2CO_2$	$r_{11} = k_{11} \cdot Fe^{2+} \cdot O_2$
r_{12}	$H_2S + 2O_2 + 2HCO_3^- \rightarrow SO_4^{2-} + 2CO_2 + 2H_2O$	$r_{12} = k_{12} \cdot (HS^- + H_2S) \cdot O_2$
r_{13}	$H_2S + HR MnO_2 + 2CO_2 \rightarrow Mn^{2+} \rightarrow S^0 + 2HCO_3^-$	$r_{13} = k_{13} \cdot (HS^- + H_2S) \cdot HR MnO_2$
r_{14}	$H_2S + PR MnO_2 + 2CO_2 \rightarrow Mn^{2+} \rightarrow S^0 + 2HCO_3^-$	$r_{14} = k_{14} \cdot (HS^- + H_2S) \cdot PR MnO_2$
r_{15}	$H_2S + 2 HR Fe(OH)_3 + 4CO_2 \rightarrow 2Fe^{2+} + S^0 + 4HCO_3^- + H_2O$	$r_{15} = k_{15} \cdot (HS^- + H_2S) \cdot HR Fe(OH)_3$
r_{16}	$H_2S + 2 MR Fe(OH)_3 + 4CO_2 \rightarrow 2Fe^{2+} + S^0 + 4HCO_3^- + H_2O$	$r_{16} = k_{16} \cdot (HS^- + H_2S) \cdot MR Fe(OH)_3$
r_{17}	$H_2S + 2 PR Fe(OH)_3 + 4CO_2 \rightarrow 2Fe^{2+} + S^0 + 4HCO_3^- + H_2O$	$r_{17} = k_{17} \cdot (HS^- + H_2S) \cdot PR Fe(OH)_3$
r_{18}	$CH_4 + CO_2 + SO_4^{2-} \rightarrow 2HCO_3^- + H_2S$	$r_{18} = k_{18} \cdot CH_4 \cdot SO_4^{2-}$
r_{19}	$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$	$r_{19} = k_{19} \cdot CH_4 \cdot O_2$
r_{20}	$FeS + O_2 \rightarrow Fe^{2+} SO_4^{2-}$	$r_{20} = k_{20} \cdot FeS \cdot O_2$
<i>Other reactions</i>		
r_{21}	$HR MnO_2 \rightarrow PR MnO_2$	$r_{21} = k_{21} \cdot HR MnO_2$
r_{22}	$HR Fe(OH)_3 \rightarrow MR Fe(OH)_3$	$r_{22} = k_{22} \cdot HR Fe(OH)_3$

Table S3. General model parameters implemented in the organic matter degradation model for the Barents Sea.

Parameter	Unit	Value	Reference
<i>Transport parameters</i>			
Length of model domain	L	cm	100
Bioirrigation coefficient	a_0	yr ⁻¹	10
Bioirrigation attenuation depth	x_{irri}	cm	3.5
Oxygen molecular diffusion coefficient	D_{O_2}	cm ² yr ⁻¹	380.44
Nitrate molecular diffusion coefficient	$D_{NO_3^-}$	cm ² yr ⁻¹	394.58
Sulfate molecular diffusion coefficient	$D_{SO_4^{2-}}$	cm ² yr ⁻¹	173.92
Ammonium molecular diffusion coefficient	$D_{NH_4^+}$	cm ² yr ⁻¹	395.87
Phosphate molecular diffusion coefficient	$D_{PO_4^{3-}}$	cm ² yr ⁻¹	112.35
Manganese molecular diffusion coefficient	$D_{Mn^{2+}}$	cm ² yr ⁻¹	123.38
Iron molecular diffusion coefficient	$D_{Fe^{2+}}$	cm ² yr ⁻¹	136.24
Hydrogen sulfide molecular diffusion coefficient	D_{H_2S}	cm ² yr ⁻¹	331.61
Porosity	φ	–	Site-specific
Bioturbation coefficient	D_{bio}	cm ² yr ⁻¹	Site-specific
Bioturbation depth	z_{bio}	cm	Site-specific
Sedimentation rate	ω	cm yr ⁻¹	Site-specific
<i>Reaction parameters</i>			
Stoichiometry constants	$x/y/z$	–	106/12/1
OM Scaling parameter	v	–	variable
OM Shaping parameter	a	yr	variable
OM reactivity – multi-G	k_{MG}	yr ⁻¹	$10^{-15} - \log(a) + 2$
OM age	age	yr	variable
Oxygen half-saturation constant	K_{O_2}	M	$8.0 \cdot 10^{-9}$
Nitrate half-saturation constant	$K_{NO_3^-}$	M	$5.0 \cdot 10^{-9}$
Manganese half-saturation constant	$K_{HR\,MnO_2}$	M	$5.0 \cdot 10^{-6}$
Iron half-saturation constant	$K_{HR\,Fe(OH)_3}$	M	$1.25 \cdot 10^{-5}$
Sulfate half-saturation constant	$K_{SO_4^{2-}}$	M	$1.0 \cdot 10^{-7}$

Table S4. Site-specific transport parameters adopted at each studied location along a 30°E S–N transect in the Barents Sea.

Parameter		Unit	B13	B14	B15	B16	B17
Porosity at sediment-water interface	φ	–	0.89	0.91	0.92	0.82	0.82
Porosity at depth	φ_∞	–	0.62	0.71	0.62	0.50	0.62
Porosity attenuation	φ_{att}	–	0.15	0.18	0.10	0.10	0.10
Bioturbation	D_{bio} [6]	$\text{cm}^2 \text{yr}^{-1}$	6.0	4.0	2.0	2.5	2.0
coefficient							
Bioturbation depth	z_{bio} [6]	cm	2	4	5	5	4
Sedimentation rate	ω [7]	cm yr^{-1}	0.05	0.05	0.06	0.05	0.05
Temperature	T [8]	°C	1.76	1.94	-1.50	-1.45	1.75
Salinity	S [8]	–	35	35	35	35	35
Water depth	h [8]	m	355	290	330	294	291

Table S5. Site-specific reaction parameters determined in this study for each studied location along a 30°E S–N transect in the Barents Sea. Parameters correspond to reaction network outlined in Table S1 and Table S2.

Parameter	Unit	B13	B14	B15	B16	B17
k_7	M ⁻¹ yr ⁻¹	$1.5 \cdot 10^7$	$1.5 \cdot 10^7$	$1.5 \cdot 10^{11}$	$1.5 \cdot 10^9$	$1.5 \cdot 10^{10}$
k_8	M ⁻¹ yr ⁻¹	$2.0 \cdot 10^8$	$2.0 \cdot 10^8$	$2.0 \cdot 10^8$	$2.0 \cdot 10^9$	$2.0 \cdot 10^{10}$
k_9	M ⁻¹ yr ⁻¹	$2.0 \cdot 10^3$				
k_{10}	M ⁻¹ yr ⁻¹	$2.0 \cdot 10^4$	$2.0 \cdot 10^4$	$2.0 \cdot 10^3$	$2.0 \cdot 10^3$	$2.0 \cdot 10^3$
k_{11}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^9$	$1.0 \cdot 10^9$	$1.0 \cdot 10^{10}$	$1.0 \cdot 10^9$	$1.0 \cdot 10^9$
k_{12}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^9$				
k_{13}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^7$				
k_{14}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^4$				
k_{15}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^7$				
k_{16}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^6$				
k_{17}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^3$				
k_{18}	M ⁻¹ yr ⁻¹	$5.0 \cdot 10^6$				
k_{19}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^{13}$				
k_{20}	M ⁻¹ yr ⁻¹	$1.0 \cdot 10^9$				
k_{21}	M ⁻¹ yr ⁻¹	$6.0 \cdot 10^{-1}$				
k_{22}	M ⁻¹ yr ⁻¹	$6.0 \cdot 10^{-1}$				

Table S6. Model-derived relative contributions of each metabolic pathway to total rates of heterotrophic organic matter degradation.

Site	Aerobic respiration %	Denitrification %	Manganese reduction %	Iron reduction %	Sulfate reduction %
B13	64.1	4.2	0.5	0.5	30.8
B14	52.6	8.3	7.3	3.1	28.7
B15	52.9	11.6	0.01	0.4	35.1
B16	74.6	3.8	2.9	0.4	18.2
B17	43.6	8.2	17.0	0.8	30.4

Table S7. Model-derived relative contributions of each transport pathway to total ammonium and phosphate benthic fluxes across the sediment-water interface.

Site	Ammonium – J_{NH4}			Phosphate – J_{PO4}				
	Diffusion %	Bioturbation %	Bioirrigation %	Advection %	Diffusion %	Bioturbation %	Bioirrigation %	Advection %
B13	59.2	1.1	39.7	<0.01	90.1	5.9	4.0	<0.01
B14	92.9	1.1	6.0	<0.01	94.3	3.9	1.8	<0.01
B15	31.2	0.2	68.6	<0.01	90.7	2.2	7.1	<0.01
B16	76.8	0.8	22.4	<0.01	93.4	3.4	3.2	<0.01
B17	82.8	0.6	16.6	<0.01	94.8	2.4	2.9	<0.01

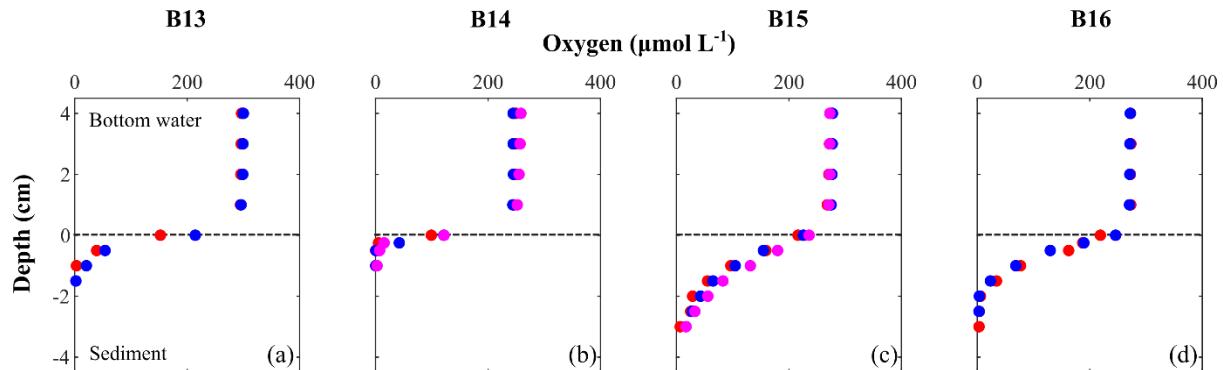


Figure S1. Oxygen concentration profiles measured in bottom waters and sediments along the 30°E S–N transect in the Barents Sea in July 2019 (RRS James Clark Ross – JR18006) [9]. Profiles were determined in 2–3 intact cores containing visually undisturbed bottom water and surface sediments from independent megacorer deployments (coloured dots) at each station. Depth profiles measured direct from cores using a *FireSting O₂-Mini sensor* (Pyro Science) mounted on a plastic support with a mobile arm which allowed data acquisition at 0.5–1.0 cm scale. Dashed line represents the sediment-water interface. No data available at B17 since this station was inaccessible at the time of sampling.

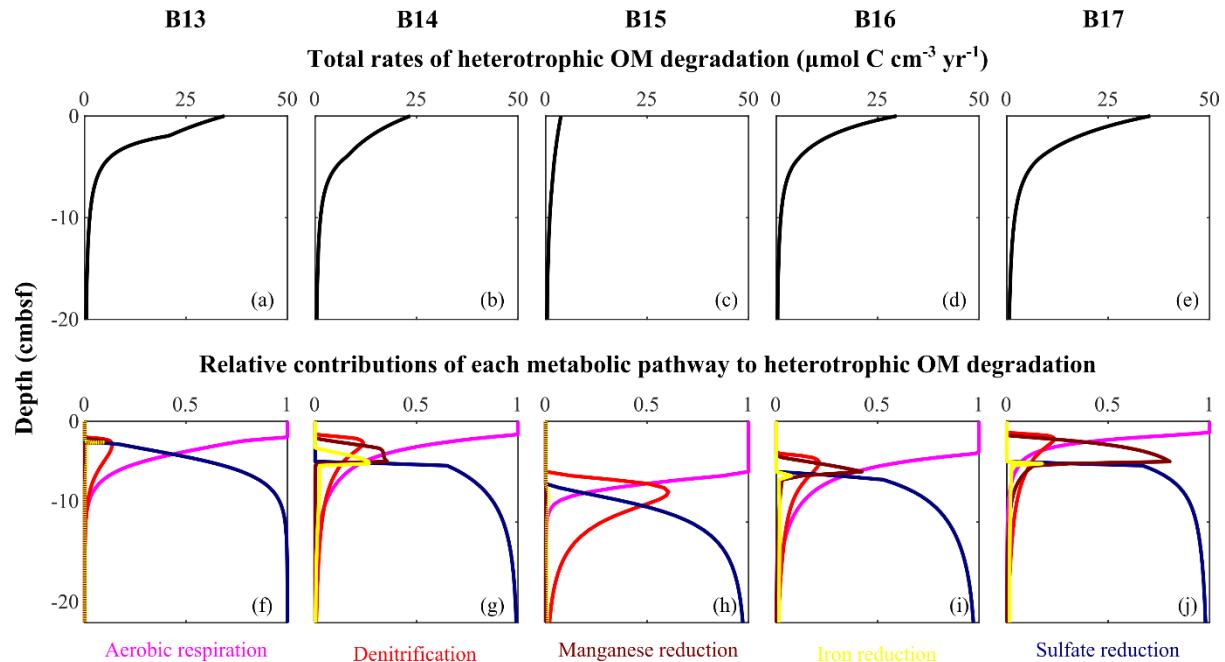


Figure S2. Depth evolution of heterotrophic organic matter degradation rates along the 30°E S–N transect in the Barents Sea. Rates are calculated assuming steady-state conditions and are derived from the primary redox reactions in Table S1 and S2. The top row (a–e) shows the depth profiles of total rates of degradation, and the bottom row (f–j) displays the depth evolution of relative contribution for each respiration pathway.

Table S8. Measured downcore concentration profiles used to inform the data-model fitting at site B13 (cruise JR16006 – July 2017).

Event	Depth cmbsf	Porewater				Event	Depth cmbsf	Sediment	
		NO_3^- μM	NH_4^+ μM	PO_4^{3-} μM	Mn^{2+} μM			TOC (R1) wt%	TOC (R2) wt%
E101	0.5	12.8	2.1	1.2	0.0	0.0	0.25	2.25	2.201
	1.5	11.9	2.3	1.3	0.0	0.0	0.75	2.061	2.002
	2.5	6.6	9.4	1.2	1.1	9.8	1.25	1.935	1.984
	4.5	0.9	30.1	1.2	1.9	56.2	1.75	1.874	
	6.5	0.6	32.6	1.1	1.3	27.8	2.5	1.829	1.946
	8.5	0.8	39.6	2.0	1.6	26.1	3.5	1.975	1.908
	10.5	1.9	24.8	1.2	2.3	26.6	4.5		1.904
	12.5	0.7	30.5	2.6	3.4	52.8	5.5	1.898	1.917
	14.5	0.9	29.7	0.7	3.2	50.6	6.5	1.776	1.796
	16.5	1.0	31.3	0.8	3.0	48.1	7.5	1.802	1.747
E102	18.5	1.0	36.6	0.5	3.2	54.1	E101	8.5	1.616
	20.5	0.6	36.7	0.4	4.0	68.7		9.5	1.525
	25.5	0.5	37.8	0.2	3.8	68.7		10.5	1.399
								11.5	1.386
	0.5	9.0	1.1	0.8	0.8	0.0		12.5	1.373
	1.5	6.4	9.2	1.8	10.9	45.2		13.5	1.361
	2.5	2.5	27.2	2.6	10.5	83.6		14.5	1.261
	4.5	1.7	41.3	1.2	8.8	79.1		15.5	1.257
	6.5	0.9	46.2	1.2	11.3	112.9		16.5	1.042
	8.5	1.3	40.2	2.2	12.6	113.0		17.5	1.24
E104	10.5	0.7	39.1	1.8	16.2	102.1		18.5	1.109
	12.5	2.0	24.7	3.0	7.3	37.9		19.5	1.212
	14.5	0.6	36.3	2.4	6.1	60.7			1.208
	16.5	0.8	36.5	2.6	5.1	43.8			
	18.5	0.7	41.8	1.5	5.6	55.2			
	20.5	0.5	44.9	0.4	5.3	64.4			
	25.5	0.7	47.5	1.1	4.7	81.3			
	0.5	9.3	1.9	0.8	0.9	0.0			
	1.5	8.6	5.3	1.8	2.7	10.1			
E104	2.5	4.0	12.7	1.8	3.6	17.4			
	4.5	0.4	40.1	1.0	4.6	67.7			
	6.5	0.7	37.4	2.3	5.2	56.1			
	8.5	0.5	35.0	3.3	6.1	37.7			
	10.5	0.6	38.2	4.2	6.8	39.4			
	12.5	0.7	35.8	3.9	8.7	40.6			
	14.5	0.5	37.3	3.9	9.0	35.4			
	16.5	0.5	39.4	4.2	9.7	20.7			
	18.5	0.5	39.7	4.7	6.2	30.7			
	20.5	0.3	40.6	3.4	4.5	33.0			
	25.5	0.7	45.1	4.1	3.5	40.3			
	30.5	0.6	47.0	3.9					

Table S9. Measured downcore concentration profiles used to inform the data-model fitting at site B14 (cruise JR16006 – July 2017).

Event	Depth cmbsf	Porewater				Event	Depth cmbsf	Sediment	
		NO_3^- μM	NH_4^+ μM	PO_4^{3-} μM	Mn^{2+} μM			TOC (R1) wt%	TOC (R2) wt%
E292	0.5	13.9	3.3	1.5	15.4		0.25	2.5	2.5
	1.5	4.6	10.3	1.2	16.9		0.75	2.3	2.4
	2.5	2.4	23.3	2.4	0.0		1.25	2.4	2.4
	4.5	2.9	22.9	1.8	0.0		1.75	2.3	2.4
	6.5	1.7	28.2	1.6	1.4		2.5	2.4	
	8.5	1.6	24.2	1.6	2.8		3.5	2.4	2.4
	10.5	1.5	22.2	1.2	2.5		4.5	2.3	2.2
	12.5	1.7	19.4	1.5	2.5		5.5	2.4	2.3
	14.5	1.5	19.8	1.9	4.6		6.5	2.2	2.1
	16.5	1.5	19.9	2.4	2.7		7.5	2.2	2.2
	18.5	1.6	26.2	3.1	2.2		8.5	2.2	2.2
	20.5	2.0	33.2	3.8	1.8		9.5	2.0	2.0
	25.5	2.0	44.0	6.4	1.4		10.5	2.1	2.0
	30.5	2.2	48.7	7.3	1.0		11.5	2.1	2.2
							12.5	2.0	2.1
E294	0.5	12.0	3.3	1.0	3.2	0.0	13.5	2.0	2.0
	1.5	6.1	14.4	1.5	49.1	32.3	14.5	2.0	2.0
	2.5	2.4	32.3	5.2	26.9	126.6	E295	15.5	1.9
	4.5	1.8	33.8	5.7	15.5	125.2		16.5	2.2
	6.5	1.4	37.3	6.2	10.1	122.8		17.5	1.9
	8.5	1.4	38.0	5.6	15.6	111.8		18.5	1.9
	10.5	1.4	34.1	7.2	6.9	99.6		19.5	1.9
	12.5	1.6	32.0	4.4	6.2	77.5		20.5	1.7
	14.5	1.5	40.9	5.2	7.3	105.3		21.5	1.7
	16.5	1.3	47.8	7.6	7.7	139.1		22.5	1.7
	18.5	1.5	49.6	6.4	8.8	126.8		23.5	1.7
	20.5	1.4	56.9	8.1	10.2	128.3		24.5	1.6
	25.5	1.6	67.9	9.0	10.3	109.9		25.5	1.7
	30.5	1.7	66.1	9.0	11.1	104.3		26.5	1.6
								27.5	1.6
E295	0.5	12.8	5.2	1.3	1.9	0.0	28.5	1.6	1.6
	1.5	5.3	19.6	3.2	31.6	91.8		29.5	1.7
	2.5	2.2	25.6	5.2	24.6	108.1		30.5	1.7
	4.5	1.6	31.6	5.9	9.6	99.8		31.5	1.6
	6.5	1.6	26.2	3.4	5.4	62.7		32.5	1.5
	8.5	1.5	25.4	3.2	3.1	55.9			
	10.5	1.7	25.6	2.8	2.8	41.6			
	12.5	2.1	24.2	3.4	3.7	34.0			
	14.5	1.6	28.4	4.8	2.5	38.2			
	16.5	1.6	32.3	4.9	2.4	34.8			
	18.5	1.5	37.5	6.2	3.0	41.9			
	20.5	1.7	38.2	6.2	2.9	38.7			
	25.5	1.5	46.4	7.9	3.5	46.3			
	30.5	1.5	50.2	8.4	3.2	45.2			

Table S10. Measured downcore concentration profiles used to inform the data-model fitting at site B15 (cruise JR16006 – July 2017).

Event	Depth cmbsf	Porewater				Event	Sediment		
		NO_3^- μM	NH_4^+ μM	PO_4^{3-} μM	Mn^{2+} μM		Depth cmbsf	TOC (R1) wt%	TOC (R2) wt%
E144	0.5	12.3	0.6	1.8	0.0	0.0	0.25	1.7	1.7
	1.5	14.0	0.3	1.9	0.0	0.0	1.25	1.7	1.8
	2.5	13.7	0.6	2.2	0.0	0.0	1.75	1.8	1.9
	4.5	7.5	0.2	2.1	5.2	0.0	2.5	1.8	1.8
	6.5	1.3	1.0	2.3	22.4	0.0	3.5	1.7	1.6
	8.5	1.9	3.4	3.1	33.8	0.0	4.5	1.6	1.6
	10.5	1.0	6.9	1.3	43.5	26.5	5.5	1.5	1.6
	12.5	2.1	7.6	0.8	38.8	49.1	6.5	1.5	1.6
	14.5	0.7	10.5	0.7	40.4	84.0	7.5	1.4	1.4
	16.5	1.8	13.5	0.5	45.4	106.1	8.5	1.4	1.5
	18.5	1.2	10.2	0.2	47.1	113.6	9.5	1.4	1.4
	20.5	0.8	22.2	0.8	107.6	102.5	10.5	1.3	1.3
	25.5	0.6	32.4	2.4	99.4	157.2	11.5	1.4	1.5
E145	30.5	0.5	35.0	1.4	106.0	168.3	12.5	1.5	1.5
							13.5	1.5	1.5
	0.5	11.0	0.2	1.2	0.0	0.0	14.5	1.5	1.4
	1.5	11.8	0.0	1.3	0.0	0.0	E144	15.5	1.5
	2.5	11.3	0.1	1.7	0.0	0.0		16.5	1.5
	4.5	8.5	0.1	2.0	10.4	0.0		17.5	1.5
	6.5	3.0	1.3	1.8	41.4	0.0		18.5	1.5
	8.5	1.7	3.8	1.3	55.4	11.9		19.5	1.5
	10.5	0.6	0.5		69.2	22.1		20.5	1.4
	12.5	0.5	13.6		59.7	35.9		21.5	1.5
	14.5	0.9	15.9		66.3	48.8		22.5	1.5
	16.5	1.0	16.3		78.1	83.0		23.5	1.5
	18.5	0.5	13.6		90.4	105.0		24.5	1.4
E146	20.5							25.5	1.5
	25.5							26.5	1.4
	30.5							27.5	1.5
								28.5	1.5
	0.5		1.7	0.3	0.0	0.0		29.5	1.4
	1.5	11.7	1.1	0.9	0.0	0.0		30.5	1.5
	2.5	13.5	3.2	1.2	0.0	0.0		31.5	1.4
	4.5	11.5	3.2	1.4	22.7	0.0		32.5	1.3
	6.5	4.5	1.5	1.4	104.7	14.9			
	8.5	1.7	6.3	1.6	82.2	0.0			
	10.5	1.6	9.8	1.7	98.3	0.0			
	12.5	1.9	10.0	1.8	93.1	0.0			
	14.5	0.9	15.0	1.5	91.3	0.0			
	16.5	0.8	17.8	1.1	70.1	192.9			
	18.5	0.7	14.8	0.5	74.4	134.6			
	20.5	1.2	23.4	0.3	74.3	105.8			
	22.5	1.1	26.6	0.1					
	25.5	1.2	19.7	0.2	75.1	78.2			
	30.5	1.3	38.9	0.2	75.1	78.2			

Table S11. Measured downcore concentration profiles used to inform the data-model fitting at site B16 (cruise JR16006 – July 2017).

Event	Depth cmbsf	Porewater				Event	Sediment		
		NO_3^- μM	NH_4^+ μM	PO_4^{3-} μM	Mn^{2+} μM		Depth cmbsf	TOC (R1) wt%	TOC (R2) wt%
E183	0.5	12.1	4.2	1.2	0.0	0.0	0.25		
	1.5	10.5	3.2	1.6	0.0	0.0	0.75	1.6	1.6
	2.5	7.1	5.7	1.3	7.1	0.0	1.25		
	4.5	2.6	15.8	2.2	26.5	77.6	1.75	1.6	1.5
	6.5	1.7	19.8	1.6	31.0	70.2	2.5	1.4	1.4
	8.5	1.3	19.4	1.9	20.5	45.8	3.5	1.4	1.4
	10.5	1.4	20.6	1.7	19.7	51.3	4.5	1.4	1.4
	12.5	1.7	21.4	1.2	17.3	54.4	5.5	1.3	1.3
	14.5	1.8	21.8	0.9	20.1	56.7	6.5		
	16.5	2.0	21.6	1.0	23.8	60.4	7.5	1.3	1.3
	18.5	1.7	23.8	0.8	22.3	64.7	8.5	1.2	1.3
	20.5	1.9	26.5	0.9	27.1	67.2	9.5	1.2	1.2
E184	25.5	1.5	32.9	1.1	25.2	97.6	10.5	1.5	1.5
	30.5	1.4	36.7	2.0	23.0	97.6	11.5	1.1	1.2
							E183	12.5	1.1
	0.5	11.5	2.6	0.9	0.0	0.0		13.5	1.1
	1.5	9.4	2.7	1.2	1.2	0.0		14.5	1.1
	2.5	8.4	4.0	1.4	8.5	0.0		15.5	1.1
	4.5	4.4	11.2	1.5	27.8	22.0		16.5	1.1
	6.5	1.4	23.6	1.5	38.4	57.7		17.5	1.1
	8.5	1.6	26.1	2.0	34.4	69.2		18.5	1.1
	10.5	1.5	31.2	1.7	28.6	81.5		19.5	1.1
	12.5	1.4	29.5	1.4	27.3	78.3		20.5	1.1
	14.5	2.0	33.7	1.3	28.4	87.9		21.5	1.0
E185	16.5	2.1	34.6	1.5	27.8	89.7		22.5	1.1
	18.5	1.3	37.6	1.4	32.9	115.4		23.5	1.0
	20.5	1.4	33.9	0.6	23.7	87.9		24.5	1.0
	25.5	1.4	34.6	0.7	24.2	81.6		25.5	1.0
								26.5	1.0
	0.5	12.2	5.2	1.1	0.0	0.0			
	1.5	8.4	3.9	1.0	0.0	0.0			
	2.5	6.4	4.7	1.3	6.2	0.0			
	4.5	1.8	25.9	1.2	17.4	54.1			
	6.5	2.3	14.9	1.1	14.9	28.7			
	8.5	1.4	19.5	0.9	18.8	43.6			
E185	10.5	5.7	24.2	1.2	16.0	61.7			
	12.5	1.7	29.8	1.2	18.5	70.0			
	14.5	1.6	29.5	0.9	20.0	70.8			
	16.5	2.2	30.7	1.2	22.4	71.0			
	18.5	2.0	33.0	1.1	23.2	76.7			
	20.5	1.3	39.0	0.8	26.0	108.1			
	25.5	1.3	37.9	1.3	27.8	111.6			

Table S12. Measured downcore concentration profiles used to inform the data-model fitting at site B17 (cruise JR16006 – July 2017).

Event	Depth cmbsf	Porewater				Event	Sediment		
		NO_3^- μM	NH_4^+ μM	PO_4^{3-} μM	Mn^{2+} μM		Depth cmbsf	TOC (R1) wt%	TOC (R2) wt%
E223	0.5	12.1	0.4	0.8	0.0	0.0	0.3	1.6	1.7
	1.5	12.5	0.4	2.0	0.0	0.0	0.5	1.7	1.8
	2.5	3.3	3.9	1.9	65.4	0.0	1.3	1.6	1.7
	4.5	1.4	16.4	3.5	108.1	110.4	1.8	1.7	1.7
	6.5	0.8	23.7	1.3	118.2	182.0	2.5	1.5	1.6
	8.5	1.2	25.3	4.3	122.1	117.0	3.5	1.4	1.5
	10.5	1.2	34.9	3.8	110.7	133.5	4.5	1.4	1.4
	12.5	1.3	33.4	3.3	97.9	196.1	5.5	1.2	1.3
	14.5	0.8	32.5	1.7	77.3	152.8	6.5	1.1	1.2
	16.5	0.9	35.0	7.8	80.5	169.4	7.5	1.1	1.2
	18.5	0.8	34.8	2.1	75.6	150.8	8.5	1.1	1.1
	20.5	1.1	33.3	2.4	72.0	126.0	9.5	1.0	1.1
E225	25.5	1.8	35.6	1.5	68.9	99.6	10.5	1.1	1.0
	30.5	0.3	14.0	0.3	53.4	125.3	11.5	1.0	1.0
	0.5	11.6	1.4	1.0	0.0	0.0	12.5	1.0	0.9
	1.5	9.8	0.5	1.7	0.0	0.0	13.5	1.0	1.0
	2.5	6.3	2.8	1.6	35.9	0.0	14.5	1.1	1.0
	4.5	0.8	21.5	2.8	102.2	184.1	15.5	1.1	1.2
	6.5	0.7	29.4	6.2	107.0	189.4	16.5	1.1	1.1
	8.5	1.0	30.1	3.1	99.8	191.6	17.5	1.0	1.1
	10.5	0.7	35.1	5.6	87.2	211.9	18.5	1.0	1.0
	12.5	1.2	40.4	2.2	79.8	212.6	19.5	0.9	0.9
	14.5	0.9	41.5	3.7	80.4	200.5	20.5	0.8	0.9
	16.5	1.5	42.7	2.7	75.1	192.8	21.5	0.9	0.9
E226	18.5	0.9	47.0	3.6	69.7	185.8	22.5	0.9	0.9
	20.5	0.9	59.8	4.1	66.1	183.6	23.5	0.9	0.9
	25.5	0.8	51.2	4.5	63.4	172.2	24.5	0.9	0.9
	30.5	1.0	50.9	3.8	62.4	158.8	25.5	0.9	0.9
	0.5	11.3	0.0	0.6	0.0	0.0	26.5	0.9	0.9
	1.5	14.0	2.3	1.2	3.0	0.0	27.5	0.8	0.8
	2.5	4.7	11.8	1.3	54.8	0.0	28.5	0.8	0.8
	4.5	1.1	18.4	2.5	180.0	57.5	29.5	0.7	0.7
	6.5	0.9	32.1	5.6	151.4	187.5	30.5	0.7	0.8
	8.5	1.0	34.5	5.0	137.3	198.6	31.5	0.7	0.8
	10.5	1.2	35.4	5.9	120.9	164.3	32.5	0.8	0.8
	12.5	1.3	43.0	2.3	98.8	224.1	33.5	0.8	0.8
	14.5	1.0	45.3	3.6	96.2	208.5			
	16.5	0.8	39.7	1.9	96.4	211.7			
	18.5	1.0	49.0	4.3	91.4	198.8			
	20.5	0.8	48.6	2.7	83.5	207.1			
	25.5	1.0	46.6	2.7	75.6	175.0			
	30.5	1.0	59.6	2.7	68.6	152.3			

References

1. Aguilera DR, Jourabchi P, Spiteri C, Regnier P. 2005 A knowledge-based reactive transport approach for the simulation of biogeochemical dynamics in Earth systems. *Geochem. Geophys. Geosystems* **6**, 1–18. (doi:10.1029/2004GC000899)
2. Thullner M, Dale AW, Regnier P. 2009 Global-scale quantification of mineralization pathways in marine sediments: A reaction-transport modeling approach. *Geochem. Geophys. Geosystems* **10**, 1–24. (doi:10.1029/2009GC002484)
3. Van Cappellen P, Wang Y. 1996 Cycling of iron and manganese in surface sediments; a general theory for the coupled transport and reaction of carbon, oxygen, nitrogen, sulfur, iron, and manganese. *Am. J. Sci.* **296**, 197–243. (doi:10.2475/ajs.296.3.197)
4. Boudreau BP, Ruddick BR. 1991 On a reactive continuum representation of organic matter diagenesis. *Am. J. Sci.* **291**, 507–538. (doi:10.2475/ajs.291.5.507)
5. Mogollón JM, Dale AW, Fossing H, Regnier P. 2012 Timescales for the development of methanogenesis and free gas layers in recently-deposited sediments of Arkona Basin (Baltic Sea). *Biogeosciences* **9**, 1915–1933. (doi:10.5194/bg-9-1915-2012)
6. Solan M, Ward ER, Wood CL, Reed AJ, Grange LJ, Godbold JA. In press. Benthic biodiversity-function relations transition across the Barents Sea Polar Front. *Phil. Trans. R. Soc. A*.
7. Zaborska A, Carroll J, Papucci C, Torricelli L, Carroll ML, Walkusz-Miotk J, Pempkowiak J. 2008 Recent sediment accumulation rates for the Western margin of the Barents Sea. *Deep Sea Res. Part II Top. Stud. Oceanogr.* **55**, 2352–2360. (doi:10.1016/j.dsr2.2008.05.026)
8. Dumont E, Brand T, Hopkins J. 2019 CTD data from NERC Changing Arctic Ocean Cruise JR16006 on the RRS James Clark Ross, Jun-August 2017. (doi:doi:10.5285/89a3a6b8-7223-0b9c-e053-6c86abc0f15d)
9. Barnes DKA. 2019 Changing Arctic Ocean Seafloor JR18006 Cruise Report. , 106.