Supplementary Information

PEATBOG: A biogeochemical model for analyzing coupled carbon and nitrogen dynamics in northern peatlands

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Supplementary Information 1 Figures

Figure 1. Graphic input in the *environmental* submodel: (a) thermal conductivity $K_{thermal}$ (m day^{-1}) change with depth, (b) the effect of air temperature on evapotranspiration rate ($f_{T,EPT}$, unitless), (c) the effects of WT depth ($f_{WT,EPT}$, unitless) (based on (Lafleur et al., 2005), Fig. 8),(d) the effect of moisture on hydraulic conductivity, (e) the relationship between WT depth (m) and water stored in the upper 1m peat, and (f) the effect of N/P ratio in moss and the uptake from deposited N in moss (fraction of total deposition). The values of (a) to (d) are listed in Table S5.

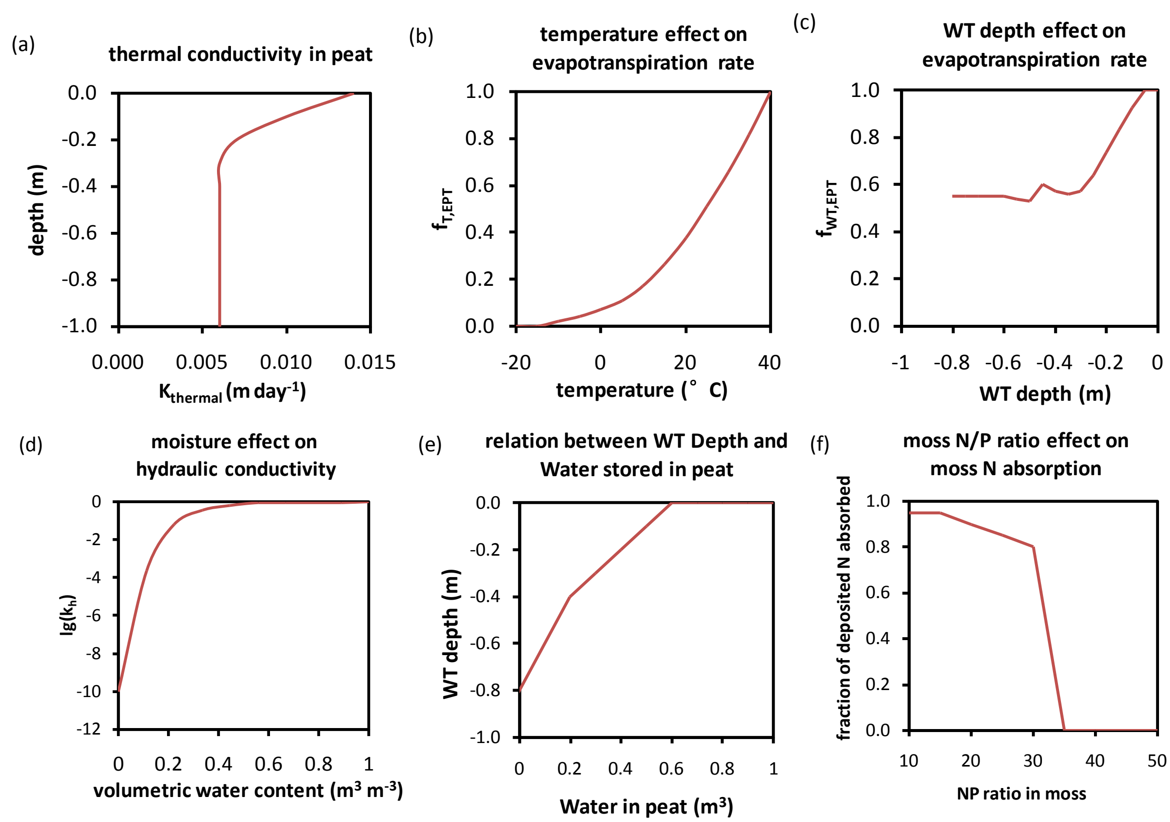


Figure 2. Graphic input in the vegetation sub-model: (a) Water table (WT) depth on the activities in shoots (am,sh, unitless) and (b) roots (am,rt, unitless), (c) the seasonal effect on moss leaf photosynthesis capacity (fseason,PSN, unitless), (d) the nitrogen and (e) temperature effect on the leaf photosynthesis capacity ($f_{N,PSNmax}$, unitless), and (f) leaf photosynthesis rate (LeafPSN, unit: umol m^{-2} s^{-1}) acclimated to incident irradiance.

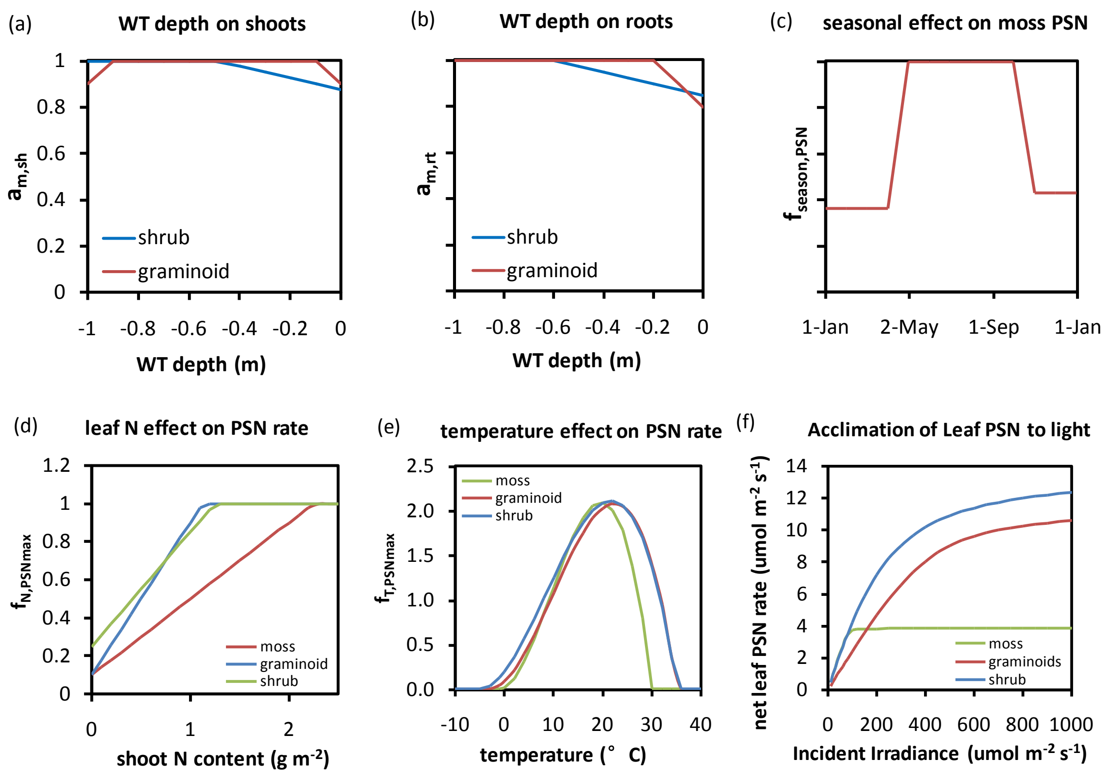


Figure 3. Graphic input in the *SOM and Dissolved* sub-models: (a) inhibition effects of dissolved CO_2 concentration (finhibi_CO_2, unitless) and (b) dissolved CH_4 concentration (finhibi_CH_4, unitless) in soil water on the decomposition rates of SOM, (c) the effect of dissolved inorganic nitrogen (DIN) on N_2 fixation rate ($f_{DIN,Nfixation}$, unitless) and (d) on mineralization and immobilization rates (fN, unitless) of soil organic matter (SOM), (e) temperature effect on the maximum CH_4 - concentration in soil above which ebullition occurs, and (f) the change of electric resistance (unit: Ω) of electron transfer in peat, redox potential (unit: V) in peat and electrical current $I_{nanowire}$ (unit: A) in peat with depth on a summer day (the dotted line indicates water table depth on that day).

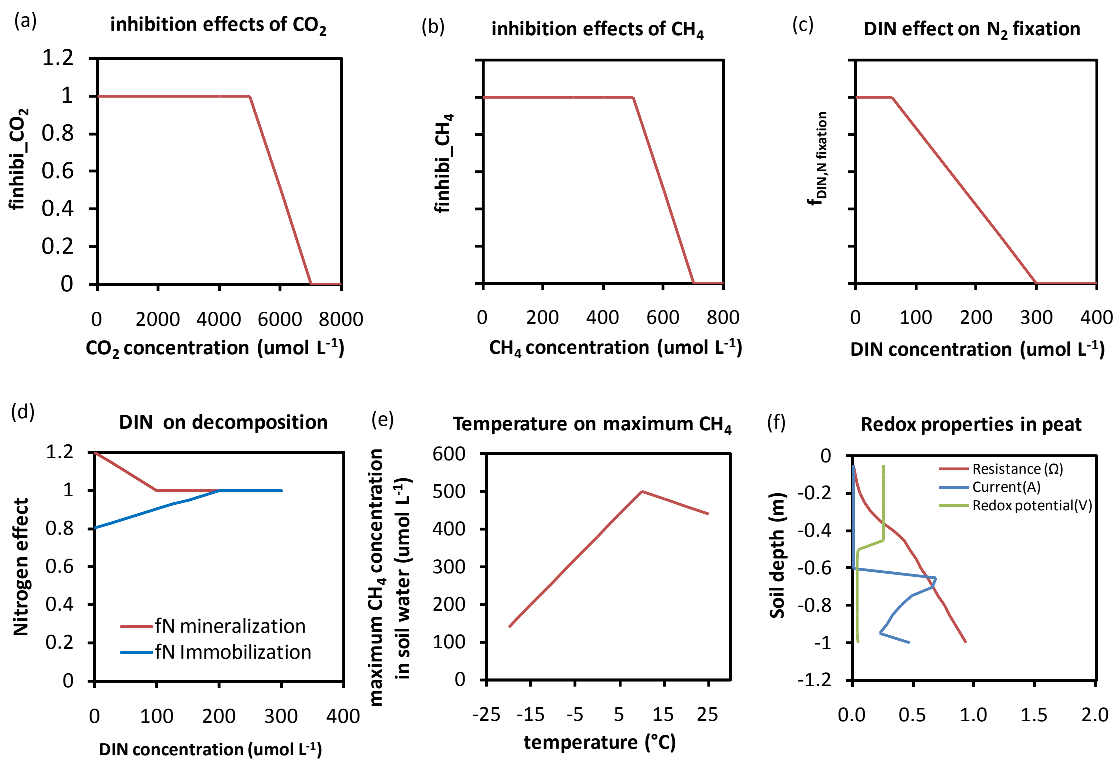
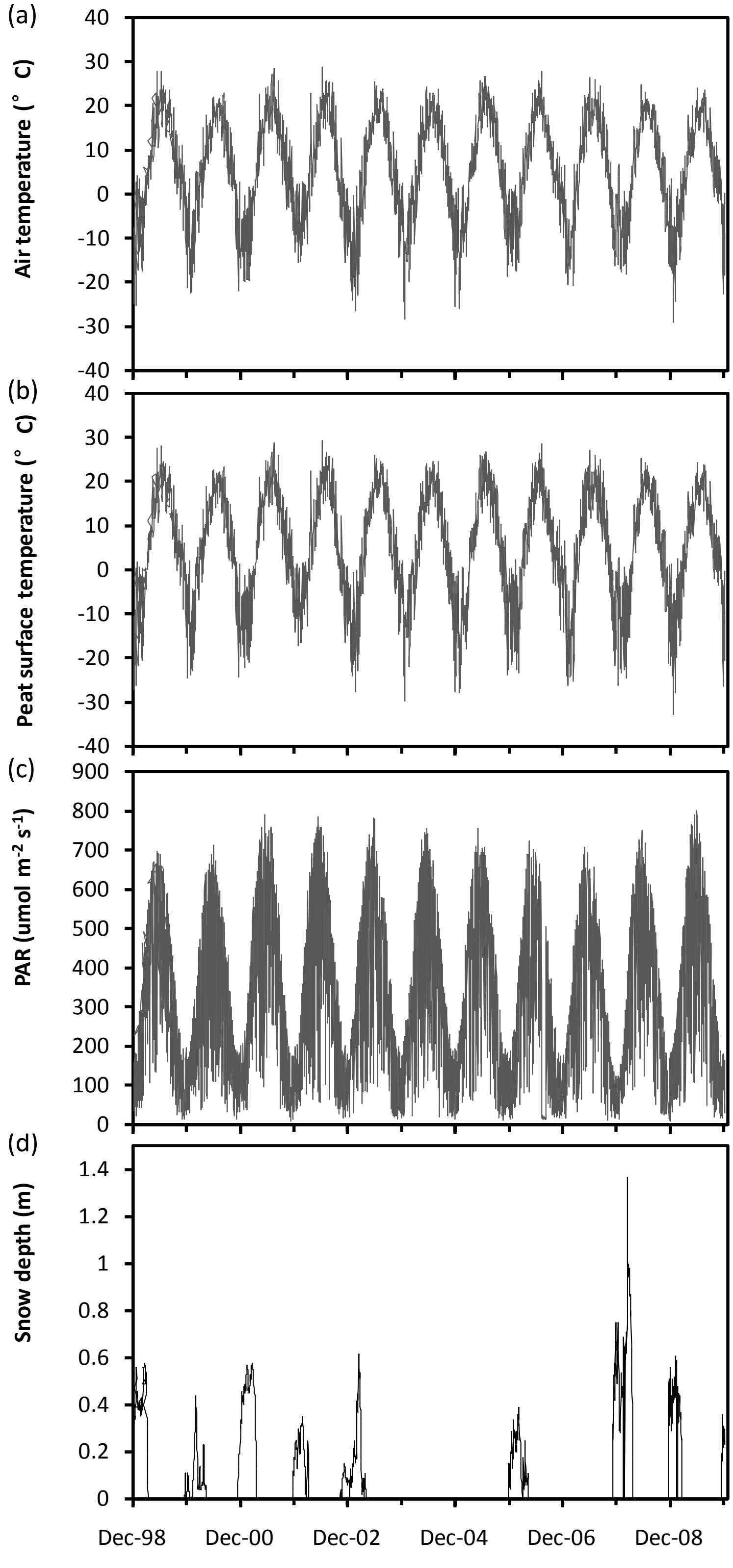


Figure 4. Environmental boundary conditions used as inputs for the model simulation of the Mer Bleue Bog from 1999 to 2009.



Supplementary information 2 Tables

Table 1 Simulated and observed estimates of annual C pools (gC m^{-2}) and C fluxes (gC m^{-2} yr^{-1}) from 1999 to 2004.

	Simulated								Observed
	1999	2000	2001	2002	2003	2004	Mean	std. Dev	
Plants C	768	753	754	751	747	732	751	11.6	
Moss C	69	70	70	68	69	70	69	0.8	66[a]
Gram. shoot C	8	8	8	8	8	8	8	0.2	4[a]
Gram. root C	19	18	18	18	18	18	18	0.1	22[a]
Shrub shoot C	119	120	117	116	114	113	117	2.5	120[a]
Shrubs root C	554	537	541	542	537	523	539	10.0	540[a]
Soil water C	1008	1020	1021	1024	1030	1034	1023	9.1	
DOC	445	446	452	457	463	457	453	7.0	
CH_4	39	40	39	39	39	40	39	0.3	
CO_2	524	534	530	528	528	538	530	4.9	
GPP	523	513	609	560	562	563	555	34.0	550[a]
GPP moss	91	135	172	151	159	167	146	29.6	120[a]
GPP Gram.	22	22	23	23	24	23	23	0.6	40[a]
GPP shrubs	410	355	414	387	379	374	386	22.4	390[a]
AR	275	242	299	283	275	247	269	22.5	250[a]
AR moss	52	74	93	82	83	88	79	14.7	44[a]
AR gram. shoot	6	6	6	6	6	6	6	0.2	
AR shrub shoot	68	52	63	60	57	49	58	7.1	
AR gram. root	8	7	7	7	7	7	7	0.5	
AR shrub root	141	103	130	128	122	95	120	17.5	
Litter	226	212	233	225	223	218	223	7.1	300[a]
Litter moss	46	43	54	50	52	51	49	4.1	55[a]
Litter vascular shoot	65	56	66	62	60	58	61	3.9	69-84[a]
Litter Gram. shoot	8	7	8	7	8	7	7	0.4	
Litter shrubs shoot	57	49	59	55	53	51	54	3.6	
Litter vascular root	115	113	113	112	111	109	112	1.9	161-176[a]
Litter Gram. root	3	3	3	3	3	3	3	0.03	
Litter shrubs root	111	110	109	109	107	106	109	1.9	
vascular plants	179	169	179	175	171	167	173	5.1	245[a]
Exudation total	62	59	85	80	76	74	73	9.8	16.5-68.8[b]
Exudation moss	8	12	26	21	26	28	20	8.2	3.6-15[b]
Exudation gram.	0	0	0	0	0	0	0	0.0	1.2-5[b]
Exudation shrubs	54	47	58	58	49	46	52	5.4	11.7-48.8[a, b]
HR	297	238	264	265	252	199	252	32.8	211[a]
CH_4 production	10	11	10	10	11	11	11	0.5	
DOC production	18	15	17	18	17	13	16	1.8	
ER	573	470	581	570	533	431	526	62.4	461[c]
NEP	-50	43	28	-9	29	133	29	61.0	40.2 (±40.5)[d]
CO_2 emission	448	339	419	421	387	288	384	60.0	
CH_4 emission	3.8	5.0	3.2	4.1	3.8	5.5	4.2	0.9	3.7 (±0.5)[d]
Plant mediated	2.7	4.4	2.6	2.8	2.8	4.7	3.3	1.0	
Ebullition	0.5	0.5	0.4	0.7	0.6	0.8	0.6	0.2	
Diffusion	0.62	0.14	0.27	0.62	0.42	0.01	0.35	0.3	
DOC export	11.0	16.8	7.8	13.8	19.0	19.5	14.6	4.7	14.9 (±3.1)[d],8.3[f]
DIC export	0.2	0.6	0.1	0.2	0.2	0.5	0.3	0.2	3.9[e]
NECB	-64.8	20.4	16.5	-27.5	5.9	107.0	9.6	57.6	21.5 (±39)[d]

[a](Moore et al., 2002); [b] (Kuzyakov, 2002); [c](Lafleur et al., 2001); [d](Roulet et al., 2007); [e](Billett and Moore, 2007); [f](Fraser et al., 2001)

Table 2 Simulated annual N pools (gN m^{-2}) and N fluxes (gN m^{-2} yr^{-1}) from 1999 to 2004.

	1999	2000	2001	2002	2003	2004	Mean	(std. Dev)
Total plant N	16.0	16.0	15.7	15.7	15.6	15.5	15.8	0.18
Moss N	1.5	1.5	1.5	1.5	1.5	1.5	1.5	0.02
Gram. N	0.6	0.6	0.6.	0.6	0.6	0.7	0.7	0.04
Gram. shoot N	0.2	0.2	0.2	0.2	0.2	0.2	0.2	0.00
Gram. root N	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.00
Shrub N	13.9	13.8	13.6	13,6	13.5	13.2	13.6	0.21
Shrub shoot N	2.5	2.5	2.4	2.4	2.3	2.3	2.4	0.09
Shrub root N	11.4	11.3	11.2	11.2	11.1	11.0	11.2	0.12
Total DIN	1.3	1.3	1.3	1.3	1.3	1.3	1.3	0.00
NH_4^+	1.3	1.3	1.3	1.3	1.3	1.3	1.3	0.00
NO_3^-	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}	10^{-7}
NO_2^-	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}	10^{-8}
Total DON	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-5}
Litter	3.9	3.7	3.9	3.8	3.8	3.7	3.8	0.11
Litter Gram. shoot	0.2	0.1	0.2	0.2	0.2	0.2	0.2	0.01
Litter shrub shoot	0.7	0.6	0.6	0.6	0.6	0.5	0.6	0.04
Litter Gram. root	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.00
Litter shrub root	2.2	2.2	2.2	2.2	2.1	2.1	2.2	0.04
Litter moss	0.8	0.8	0.9	0.8	0.8	0.8	0.8	0.05
Exudation	0.04	0.06	0.05	0.04	0.04	0.04	0.04	0.01
Exudation moss	0.01	0.04	0.02	0.01	0.01	0.02	0.02	0.01
Exudation Gram.	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Exudation shrub	0.03	0.02	0.03	0.03	0.03	0.02	0.03	0.00
N mineralization	2.2	1.6	2.0	2.1	2.0	1.4	1.9	0.30
DON production	0.6	0.5	0.5	0.6	0.5	0.4	0.5	0.07
N uptake	1.8	1.6	1.8	1.8	1.7	1.4	1.7	0.18
Graminoids DIN	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.01
Shrubs DIN	1.7	1.5	1.7	1.6	1.6	1.2	1.6	0.17
Graminoids DON	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.00
Shrubs DON	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}	10^{-4}
N inception mosses	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.00
N through fall	0.04	0.04	0.04	0.04	0.04	0.04	0.04	0.00
N2 fixation	1.0	1.0	1.0	1.0	1.0	1.0	1.0	0.00
DON export	0.03	0.04	0.02	0.02	0.02	0.08	0.04	0.02
DIN export	0.00	0.01	0.00	0.00	0.01	0.01	0.01	0.00
N sequestration in peat	1.2	1.7	1.4	1.2	1.3	1.9	1.4	0.28

Table 3 Changes in simulated carbon and nitrogen cycling components due to the change of air temperature (Air T), precipitation (*Pre*), annual nitrogen deposition (N, unit gN·m^{-2}·yr^{-1}) and parameters: temperature effect on the decomposition of labile *(L)* and recalcitrant ($Q_{10,R}$), potential decomposition constant of labile soil (k_{Lpot}) and of recalcitrant soil ($k_{R,pot}$). The changes are expressed in percentages relative to the baseline simulations. Negative signs indicate decreases relative to the baseline and positive signs indicate increases.

	GPP	AR	NPP moss	NPP Gram	NPP shrub	HR	CH_4	ER	DOC	DIC	NEE	NECB	ΔC SOM	ΔN SOM
Air T (-1)	-2	-4	0	-2	0	-7	+4	-6	0	+16	+65	+228	+70	+1
Air T (+1)	+2	+4	-3	-1	0	+7	-6	+6	-1	-13	-72	+251	-81	-2
Air T (+3)	+3	+12	-14	-13	-1	+20	-18	+17	-5	-32	-232	-810	-275	-10
Air T (+5)	+4	+20	-34	+11	-3	+32	-23	+28	-11	-46	-416	-1450	-497	-19
Pre (-30%)	+1	+6	0	+6	-4	+11	-25	+9	-36	-66	-148	-443	-231	-46

Pre (-15%)	+1	+3	0	+3	-2	+5	-10	+5	-14	-38	-69	-214	-100	-19
Pre (+15%)	-1	-2	+1	-3	+1	-4	+13	-3	+9	+52	+36	+106	+80	+15
Pre (+30%)	-1	-4	+1	-5	+2	-7	+19	-6	+14	+108	+87	+273	+146	+27
N (0.2)	-18	-30	+5	-28	-11	-6	-1	-18	+8	+45	-28	-114	+81	-45
N (1.4)	+9	+17	-20	+30	+8	0	+5	+8	-3	-10	+22	+80	-14	+59
N (2.0)	+13	+19	-23	+70	+13	0	+12	+9	-3	-10	+71	+252	+41	+115
N (2.6)	+16	+26	-43	+260	+12	-1	+22	+12	-4	-14	+93	+327	+106	+190
N (3.2)	+19	+31	-59	+560	+4	-2	+32	+14	-5	-16	+122	-141	+189	+251
$Q_{10,R}$ (2)	-1	-1	-100	-100	-100	-14	-13	-8	-8	-4	+128	+480	+277	+31
$Q_{10,L}$ (3.3)	0	0	+1	0	0	0	0	0	+6	+3	0	+4	-51	-1
k_{Rpot}(+25%)	+1	+2	+54	-13	+2	+20	+26	+11	+13	+11	-175	-667	-399	-45
k_{Rpot}(-25%)	-2	-2	-4	+1	+7	-22	-26	-12	-14	-13	+186	+707	+430	+44
k_{Lpot}(+25%)	0	0	-100	-100	-100	+6	+1	+3	+5	-1	-50	-187	-110	-12
k_{Lpot}(-25%)	0	0	-100	-100	-100	-7	-2	-4	-5	-1	+62	-137	+136	+10

Table 4 Initials for the initialization simulations. The initials values of C and N pools were calculated from bulk density at each layer depth and C/N ratio (Blodau and Moore, 2002; Blodau et al., 2006). The fraction of labile and recalcitrant was assumed based on (Bridgham et al., 1998). The initial concentration of CO_2, CH_4 and H_2 were assumed based on (Beer and Blodau, 2007).

Layer	SOM labile C (g)	SOM recalcitrant C (g)	SOM labile N (g)	SOM recalcitrant N (g)	CO_2 concentration (mmol m^{-3})	CH_4 concentration (mmol m^{-3})	H_2 concentration (nmol L^{-1})
1	266.5	1066.0	5.8	23.2	0	0	20
2	236.9	1737.2	5.0	37.0	0	0	20.5
3	248.4	2235.8	4.7	42.2	0	0	21
4	234.0	2690.4	4.1	47.2	0	0	21.5
5	232.3	3086.5	4.1	55.1	0	0	22
6	220.8	3459.5	4.8	75.2	0	0	22.5
7	200.8	3815.6	5.0	95.4	500	50	23
8	173.3	4159.1	4.4	106.6	1000	100	23.5
9	138.9	4492.6	3.8	121.4	1500	150	24
10	98.3	4818.3	3.0	146.0	2000	200	24.5
11	77.8	5111.8	2.5	164.9	2500	250	26
12	54.5	5397.6	1.9	186.1	3000	300	30
13	28.5	5676.7	0.8	149.4	3500	350	40
14	11.9	5938.2	0.3	148.5	4000	400	50
15	6.2	6181.3	0.2	154.5	4500	450	55
16	5.8	6412.3	0.1	160.3	5000	500	60
17	5.3	6637.2	0.1	165.9	5000	500	70
18	4.1	6857.2	0.1	171.4	5000	500	80
19	2.8	7072.1	0.1	176.8	5000	500	90
20	174.8	873875.2	4.4	21846.9	5000	500	100

Units were standardized to 1 m^2 area of peatlands for model output.

Table 5 Parameter values in Figure S1

Layer depth (m)	0	-0.1	-0.2	-0.3	-0.4	-0.5	-0.6	-0.7	-0.8	-0.9	-1.0
Thermal conductivity ($K_{thermal,0}$) (m s^{-1})	0.014	0.01	0.007	0.006	0.006	0.006	0.006	0.006	0.006	0.006	0.006

Air temperature (°C)	below -15	-10	-5	-0	5	10	15	20	25	30	35	40

Effect of temperature on evapotranspiration rate (unitless)	0	0.02	0.04	0.07	0.11	0.17	0.265	0.375	0.51	0.655	0.815	1

Water table depth (m)	below -0.5	-0.5	-0.45	-0.4	-0.35	-0.3	-0.25	-0.2	-0.15	-0.1	above -0.1
Effect of WT depth on evapotranspiration rate (unitless)	0.55	0.53	0.6	0.57	0.56	0.57	0.64	0.738	0.832	0.927	1

Volumetric water content (m^3 m^{-3})	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1
log value of hydraulic conductivity (unitless)	-10	-4.04	-1.52	-0.58	-0.26	-0.13	-0.06	-0.05	-0.05	-0.05	0

Table 6 Parameters for Henry's law, Fick's law and electron flows

Parameter	Description	Value	Unit	Source
$K_{H,DMg,0}$	Henry's constant of dissolved gas (DM_g) at 25 ºC	$K_{H,CO2}$ = 0.034 $K_{H,CH4}$= 0.014 $K_{H,O2}$= 0.013	mol L^{-1} atm^{-1}	(Sander, 1999)
$C_{H,inv,DMg}$	Henry's law coefficient	$C_{H,inv,CH4}$ = 1600 $C_{H,inv,CO2}$ = 2400 $C_{H,inv,O2}$ = 1500		(Sander, 1999)
$D_{DMS,0}$	Standard diffusion coefficient of solutes	D_{DOM} = $1.19 \cdot 10^{-5}$ D_{NO3} =$1.69 \cdot 10^{-4}$ D_{NH4}= $8.47 \cdot 10^{-5}$	m^2 day^{-1}	(Krom and Berner, 1980, Jones et al., 2005, Van Rees et al. 2003)
$D_{DMg,0}$	Standard diffusion coefficient of gases	D_{CO2} = $1.51 \cdot 10^{-4}$ D_{CH4}= $1.36 \cdot 10^{-4}$ D_{O2} =$1.56 \cdot 10^{-4}$	m^2 day^{-1}	(Broecker and Peng, 1974; Cornel et al., 1986; Fredlund et al., 1993)
C	Coulombs, the magnitude of electrical charge in protons of electrons	$6.2415 \cdot 10^{18}$	e^- electron $proton^{-1}$	SI
N_A	Avogadro constant	$6.02 \cdot 10^{23}$	mol^{-1}	SI
F	Faraday constant	96490	Coulombs mol^{-1}	The NIST Reference on Constants, Units and Uncertainty
$\Delta G^0_{r,i}$	standard change of reaction in Gibbs free energy	-193.1	kJ mol^{-1}	(Nordstrom and Munoz,1994; (Stumm and Morgan))
R	gas constant	8.13	J K^{-1} mol^{-1}	

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