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Coupled eco-hydrology and biogeochemistry algorithms enable the simulation of water table depth effects on boreal peatland net CO_2 exchange

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Supplementary material

Appendix A: Soil carbon (C), nitrogen (N) and phosphorus (P) transformations

Decomposition

$D_{Si,j,l,\mathrm{C}} = D'_{Si,j,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\;\; f_{\mathrm{tg}l}\, (S_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of litter, POC, humus	[SA1a]
$D_{Zi,j,l,\mathrm{C}} = D'_{Zi,j,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\; f_{\mathrm{tg}l}\, (Z_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of microbial residues	[SA1b]
$D_{Ai,l,\mathrm{C}} = D'_{Ai,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\; f_{\mathrm{tg}l}\, (A_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of adsorbed SOC	[SA1c]
$S_{i,l,\mathrm{C}} = \Sigma_j\, S_{i,j,l,\mathrm{C}}$	total C in all kinetic components of litter, POC, humus	[SA2a]
$Z_{i,l,\mathrm{C}} = \Sigma_j\, Z_{i,j,l,\mathrm{C}}$	total C in all kinetic components of microbial residues	[SA2b]
$G_{i,l,\mathrm{C}} = S_{i,l,\mathrm{C}} + Z_{i,l,\mathrm{C}} + A_{i,l,\mathrm{C}}$	total C in substrate-microbe complexes	[SA2c]
$M_{i,d,l,\mathrm{C}} = M_{i,a,l,\mathrm{C}} + \boldsymbol{q_m}\, (M_{i,a,l,\mathrm{C}}\, G_{ix,l,\mathrm{C}} - M_{ix,a,l,\mathrm{C}}\, G_{i,l,\mathrm{C}})/(G_{ix,l,\mathrm{C}} + G_{i,l,\mathrm{C}})$	redistribution of active microbial biomass from each substrate-microbe complex *i* to other substrate-microbe complexes *ix* according to concentration differences (priming)	[SA3a]
$M_{i,a,l,\mathrm{C}} = \Sigma_n\, M_{i,n,a,l,\mathrm{C}}$		[SA3b]
$D'_{Si,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Sj,\mathrm{C}}[S_{i,j,l,\mathrm{C}}]\}/\{[S_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [\Sigma M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$	substrate and water constraint on *D* from colonized litter, POC and humus, microbial residues and adsorbed SOC	[SA4a]
$D'_{Zi,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Zj,\mathrm{C}}[Z_{i,j,l,\mathrm{C}}]\}/\{[Z_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$		[SA4b]
$D'_{Ai,l,\mathrm{C}} = \{\boldsymbol{D}_{A,\mathrm{C}}[A_{i,l,\mathrm{C}}]\}/\{[A_{i,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$		[SA4c]
$\delta S_{i,j,k,l,\mathrm{C}}/\delta t = \boldsymbol{\beta}\, \Sigma_n\, (U_{i,n,l\mathrm{C}} - R_{\mathrm{h}i,n,l})\, (S'_{i,j,k,l,\mathrm{C}}/ S'_{i,j,l,\mathrm{C}})\; \{(S'_{i,j,l,\mathrm{C}}/S_{i,j,l,\mathrm{C}})/(S'_{i,j,l,\mathrm{C}}/S_{i,j,l,\mathrm{C}} + \boldsymbol{K}_{\mathbf{i}\boldsymbol{S}})\}$	colonized litter determined by microbial growth into uncolonized litter	[SA5]
$f_{\mathrm{tg}l} = T_{\mathrm{s}l}\{e^{[B - \boldsymbol{H}_{\mathbf{a}}/(\boldsymbol{R}T_{\mathrm{s}l})]}\}/\{1 + e^{[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{s}l})/(\boldsymbol{R}T_{\mathrm{s}l})]} + e^{[(\boldsymbol{S}T_{\mathrm{s}l} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{s}l})]}\}$	Arrhenius function for *D* and R_{h}	[SA6]

$D_{Si,j,l,\mathrm{N,P}} = D_{Si,j,l,\mathrm{C}}(S_{i,j,l,\mathrm{N,P}}/S_{i,j,l,\mathrm{C}})$	N and P coupled with C during D	[SA7a]
$D_{Zi,j,l,\mathrm{N,P}} = D_{Zi,j,l,\mathrm{C}}(Z_{i,j,l,\mathrm{N,P}}/Z_{i,j,l,\mathrm{C}})$		[SA7b]
$D_{Ai,l,\mathrm{N,P}} = D_{Ai,l,\mathrm{C}}(A_{i,l,\mathrm{N,P}}/A_{i,l,\mathrm{C}})$		[SA7c]
$Y_{i,l,\mathrm{C}} = \boldsymbol{k}_{\mathbf{ts}}(G_{i,l,C}\, F_{\mathrm{s}}[Q_{i,l,\mathrm{C}}]^{\boldsymbol{b}} - X_{i,l,\mathrm{C}})$	Freundlich sorption of DOC	[SA8]
$Y_{i,l,\mathrm{N,P}} = Y_{i,l,\mathrm{C}}(Q_{i,l,\mathrm{N,P}}/Q_{i,l,\mathrm{C}})$	($Y_{i,l,\mathrm{C}} > 0$) adsorption of DON, DOP	[SA9]
$Y_{i,l,\mathrm{N,P}} = Y_{i,l,\mathrm{C}}(X_{i,l,\mathrm{N,P}}/X_{i,l,\mathrm{C}})$	($Y_{i,l,\mathrm{C}} < 0$) desorption of DON, DOP	[SA10]

Microbial growth

$R_{\mathrm{h}} = \Sigma_i\Sigma_n\Sigma_l R_{\mathrm{h}i,n,l}$		[SA11]
$\boldsymbol{R}_{\mathrm{h}i,n,l} = \boldsymbol{R'}_{\mathrm{h}n} \min\{C_{\mathrm{N}i,n,l,a}/\boldsymbol{C}_{\mathbf{N}j},\, C_{\mathrm{P}i,n,l,a}/\boldsymbol{C}_{\mathbf{P}j}\}$	R_{h} constrained by microbial N, P	[SA12]
$R_{\mathrm{h}}'_{i,n,l} = M_{i,n,a,l,\mathrm{C}}\ \{\boldsymbol{R}_{\mathrm{h}i,n,l}\,[Q_{i,l,\mathrm{C}}]\}/\{(\boldsymbol{K}_{\mathbf{m}\boldsymbol{Q}\mathbf{C}} + [Q_{i,l,\mathrm{C}}])\}f_{\mathrm{tg}l}\, f_{\psi gl}$	R_{h} constrained by substrate DOC	[SA13]
$R_{\mathrm{h}i,n,l} = R_{\mathrm{h}}'_{i,n,l}\,(U_{\mathrm{O2}i,n,l}/U'_{\mathrm{O2}i,n,l})$	R_{h} constrained by O_2	[SA14]
$f_{\psi gl} = 1.0 - 6.67(1.0 - e^{(M\psi_{\mathrm{s}}/(\boldsymbol{R}T_{\mathrm{s}l})})$	ψ_{s} constraints on microbial growth	[SA15]
$U'_{\mathrm{O2}i,n,l} = 2.67 R_{\mathrm{h}}'_{i,n,l}$	O_2 demand driven by potential R_{h}	[SA16]
$U_{\mathrm{O2}i,n,l} = U'_{\mathrm{O2}i,n,l}[\mathrm{O}_{2\mathrm{m}i,n,l}]/([\mathrm{O}_{2\mathrm{m}i,n,l}] + \boldsymbol{K}_{\mathbf{O_2}})$	active uptake coupled with radial diffusion of O_2	[SA17a]
$= 4\pi n\, M_{i,n,a,l,\mathrm{C}}\, D_{\mathrm{sO2}l}[\boldsymbol{r}_{\mathbf{m}} r_{\mathrm{w}l}/(r_{\mathrm{w}l} - \boldsymbol{r}_{\mathbf{m}})]([\mathrm{O}_{2\mathrm{s}l}] - [\mathrm{O}_{2\mathrm{m}i,n,l}]$		[SA17b]
$R_{\mathrm{m}i,n,j,l} = \boldsymbol{R}_{\mathrm{m}} M_{i,n,j,l,\mathrm{N}} f_{\mathrm{tm}l}$		[SA18]
$f_{\mathrm{tm}l} = e^{[\boldsymbol{y}(T_{\mathrm{s}l} - 298.16)]}$		[SA19]
$R_{\mathrm{g}i,n,l} = R_{\mathrm{h}i,n,l} - \Sigma_j\, R_{\mathrm{m}i,n,j,l}$		[SA20]
$U_{i,n,l\mathrm{C}} = \min(R_{\mathrm{h}i,n,l}\,,\, \Sigma_j\, R_{\mathrm{m}i,n,j,l}) + R_{\mathrm{g}i,n,l}\,(1 + \boldsymbol{\Delta G_x}/\boldsymbol{E}_{\mathbf{m}})$	DOC uptake driven by R_{g}	[SA21]
$U_{i,n,l\mathrm{N,P}} = U_{i,n,l} Q_{i,l,\mathrm{N,P}}/Q_{i,l,\mathrm{C}}$	DON,DOP uptake driven by $U_{i,n,l\mathrm{C}}$	[SA22]
$D_{Mi,n,j,l,\mathrm{C}} = \boldsymbol{D}_{Mi,j} M_{i,n,j,\mathrm{C}} f_{\mathrm{tg}}$	first-order decay of microbial C,	[SA23]

$D_{Mi,n,j,\mathrm{N,P}} = \boldsymbol{D}_{Mi,j} M_{i,n,j,l,\mathrm{N,P}} f_{\mathrm{tg}l}\, f_{\mathrm{d}i,n,l\mathrm{N,P}}$ partial release of microbial N, P [SA24]

$\delta M_{i,n,j,l,\mathrm{C}}/\delta t = F_j\, U_{i,n,l\mathrm{C}} - F_j R_{\mathrm{h}i,n,l} - D_{Mi,n,j,l,\mathrm{C}}$ $[R_{\mathrm{h}i,n,l} > R_{\mathrm{m}i,n,j,l}]$ growth [SA25a]

$\delta M_{i,n,j,l,\mathrm{C}}/\delta t = F_j\, U_{i,n,l\mathrm{C}} - R_{\mathrm{m}i,n,j,l} - D_{Mi,n,j,l,\mathrm{C}}$ $[R_{\mathrm{h}i,n,l} < R_{\mathrm{m}i,n,j,l}]$ senescence [SA25b]

Microbial nutrient exchange

$U_{\mathrm{NH4}i,n,j,l} = (M_{i,n,j,l,C}\, \boldsymbol{C}_{\mathbf{N}j} - M_{i,n,j,l,N})$ $U_{\mathrm{NH_4}} < 0$ mineralization [SA26a]

$U_{\mathrm{NH_4}i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}j} - M_{i,n,j,l,N}),$
$\boldsymbol{U'}_{\mathbf{NH_4}}\, a_{i,n,j,l}\, ([\mathrm{NH_4}^+{}_{i,n,j,l}] - [\mathbf{NH_4^+}_{\mathbf{mn}}])/([\mathrm{NH_4}^+{}_{i,n,j,l}] - [\mathbf{NH_4^+}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\}$ $U_{\mathrm{NH_4}} > 0$ immobilization [SA26b]

$U_{\mathrm{NO_3}i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}j} - (M_{i,n,j,l,N} + U_{\mathrm{NH_4}i,n,j,l}))\ ,$
$\boldsymbol{U'}_{\mathbf{NO_3}}\, a_{i,n,j,l}\, ([\mathrm{NO_3}^-{}_{i,n,j,l}] - [\mathbf{NO_3^-}_{\mathbf{mn}}])/([\mathrm{NO_3}^-{}_{i,n,j,l}] - [\mathbf{NO_3^-}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\}$ $U_{\mathrm{NO_3}} > 0$ immobilization [SA26c]

$U_{\mathrm{PO4}i,n,j,l} = (M_{i,n,j,l,C}\, \boldsymbol{C}_{\mathbf{P}j} - M_{i,n,j,l,P})$ $U_{\mathrm{PO_4}} < 0$ mineralization [SA26d]

$U_{\mathrm{PO4}i,n,j,l} = \min\{(M_{i,n,j,l,C}\, \boldsymbol{C}_{\mathbf{P}j} - M_{i,n,j,l,P}),$
$\boldsymbol{U'}_{\mathbf{PO_4}}\, A_{\ i,n,j,l}\, ([\mathrm{H_2PO_4}^-{}_{i,n,j,l}] - [\mathbf{H_2PO_4^-}_{\mathbf{mn}}])/([\mathrm{H_2PO_4}^-{}_{i,n,j,l}] - [\mathbf{H_2PO_4^-}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{PO_4}})\}$ $U_{\mathrm{PO_4}} > 0$ immobilization [SA26e]

$\Phi_{i,n=f,j,l} = max\{0, M_{i,n=f,j,l,\mathrm{C}} \boldsymbol{C}_{\mathbf{N}j} - M_{i,n=f,j,l,\mathrm{N}} - max\{0, U_{i,n=f,j,l,\mathrm{N}}\}\}$ N_2 fixation driven by N deficit of diazotrophic population [SA27]

$R_{\Phi i,n=f,j,l} = \boldsymbol{E}_{\boldsymbol{\Phi}}\, \Phi_{i,n=f,j,l}$ [SA28]

$\delta M_{i,n,j,l,\mathrm{N}}/\delta t = F_j U_{i,n,l,\mathrm{N}} + U_{\mathrm{NH_4}i,n,j,l} + U_{\mathrm{NO_3}i,n,j,l} + \Phi_{i,n=f,j,l} - D_{Mi,n,j,l,\mathrm{N}}$ growth *vs*. losses of microbial N, P [SA29a]

$\delta M_{i,n,j,l,\mathrm{P}}/\delta t = F_j U_{i,n,l,\mathrm{P}} + U_{\mathrm{PO_4}i,n,j,l} - D_{Mi,n,j,l,\mathrm{p}}$ [SA29b]

$M_{i,n,a,l,\mathrm{C}} = M_{i,n,j=labile,l,\mathrm{C}} + M_{i,n,j=resistant,l,\mathrm{C}} F_{\mathrm{r}}/F_{\mathrm{l}}$ [SA30]

Humification

$H_{Si,j=\mathrm{lignin},l,\mathrm{C}} = D_{Si,j=\mathrm{lignin},l,\mathrm{C}}$ decomposition products of litter added to POC depending on lignin [SA31]

$H_{Si,j=\mathrm{lignin},l,\mathrm{N,P}} = D_{Si,j=\mathrm{lignin},l,\mathrm{N,P}}$ [SA32]

$H_{Si,j\neq\mathrm{lignin},l,\mathrm{C}} = H_{Si,j=\mathrm{lignin},l,\mathrm{C}}\, \boldsymbol{L}_{\mathbf{h}j}$ [SA33]

$H_{Si,j\neq\mathrm{lignin},l,\mathrm{N,P}} = H_{Si,j\neq\mathrm{lignin},l,\mathrm{C}}\, S_{i,l,\mathrm{N,P}}/S_{i,l,\mathrm{C}}$ [SA34]

$H_{Mi,n,j,l,C} = D_{Mi,n,j,l,C}\,\boldsymbol{F}_{\mathbf{h}}$	decomposition products of microbes added to humus depending on clay	[SA35]
$H_{Mi,n,j,l,N,P} = H_{Mi,n,j,l,C} M_{i,n,j,l,N,P} / M_{i,n,j,l,C}$		[SA36]

Definition of variables in Appendix A

Variable	Definition	Unit	Value	Reference
	Subscripts			
i	substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus			
j	kinetic component: labile l, resistant r, active a			
l	soil or litter layer			
n	microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)			
	Variables			
$A_{i,l,C}$	mass of adsorbed SOC	g C m^{-2}		
$[A_{i,l,C}]$	concentration of adsorbed SOC in soil	g C Mg^{-1}		
a	microbial surface area	m^2 m^{-2}		
$\boldsymbol{B}$	parameter such that f_{tg} = 1.0 at T_l = 298.15 K		26.230	
$\boldsymbol{b}$	Freundlich exponent for sorption isotherm		0.85	(Grant et al., 1993a, b)
$\boldsymbol{\beta}$	specific colonization rate of uncolonized substrate	-	2.5	(Grant et al., 2010)
$C_{N,Pi,n,a,l}$	ratio of $M_{i,n,a,N,P}$ to $M_{i,n,a,C}$	g N or P g C^{-1}		
$\boldsymbol{C}_{\mathbf{N,P}j}$	maximum ratio of $M_{i,n,j,N,P}$ to $M_{i,n,j,C}$ maintained by $M_{i,n,j,C}$	g N or P g C^{-1}	0.22 and 0.13 (N), 0.022 and 0.013 (P) for j = labile and resistant, respectively	(Grant et al., 1993a, b)

$\boldsymbol{D}_{Mi,j}$	specific decomposition rate of $M_{i,n,j}$ at 30°C	g C g C^{-1} h^{-1}	0.0125 and 0.00035 for j = labile and resistant, respectively	(Grant et al., 1993a, b)
$D_{Mi,n,j,l,\mathrm{C}}$	decomposition rate of $M_{i,n,j,l,\mathrm{C}}$	g C m^{-2} h^{-1}		
$D_{Mi,n,j,l,\mathrm{N,P}}$	decomposition rate of $M_{i,n,j,l,\mathrm{N,P}}$	g N or P m^{-2} h^{-1}		
$D_{\mathrm{sO2}l}$	aqueous dispersivity–diffusivity of O_2 during microbial uptake in soil	m^2 h^{-1}		
$D_{Ai,l,\mathrm{C}}$	decomposition rate of $A_{i,l,\mathrm{C}}$ by $M_{\boldsymbol{i,d,l},\mathrm{C}}$ producing Q [SA13]	g C m^{-2} h^{-1}		
$\boldsymbol{D}_{Aj,\mathrm{C}}$	specific decomposition rate of $A_{i,l,\mathrm{C}}$ by $M_{\boldsymbol{i,d,l},\mathrm{C}}$ at 25°C and saturating[$A_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	0.025	(Grant et al., 1993a, b)
$D_{Ai,j,\,l,\mathrm{N,P}}$	decomposition rate of $A_{i,l,\mathrm{N,P}}$ by $M_{\boldsymbol{i,d,l},\mathrm{C}}$	g N or P m^{-2} h^{-1}		
$D'_{Ai,j,\,l,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}		
$D_{Si,j,l,\mathrm{C}}$	decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ producing Q [SA13]	g C m^{-2} h^{-1}		
$\boldsymbol{D}_{Sj,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[$S_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	1.0, 1.0, 0.15, and 0.025 for j = protein, carbohydrate, cellulose, and lignin	(Grant et al., 1993a, b)
$D_{Si,j,\,l,\mathrm{N,P}}$	decomposition rate of $S_{i,j,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m^{-2} h^{-1}		
$D'_{Si,j,\,l,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}		
$D_{Zi,j,l,\mathrm{C}}$	decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ producing Q in [SA13]	g C m^{-2} h^{-1}		
$D_{Zi,j,\mathrm{N,P}}$	decomposition rate of $Z_{i,j,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m^{-2} h^{-1}		
$\boldsymbol{D}_{Zj,\mathrm{C}}$	specific decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[$Z_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	0.25 and 0.05 for j = labile and resistant biomass	(Grant et al., 1993a, b)
$D'_{Zi,j,l,\mathrm{C}}$	specific decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}		

$\boldsymbol{\Delta G_x}$	energy yield of C oxidation with different reductants x	kJ g C^{-1}	37.5 ($x = O_2$); 4.43 (x = DOC)	
$\boldsymbol{E_m}$	energy requirement for growth of $M_{i,n,a,l}$	kJ g C^{-1}	25	
$\boldsymbol{E_\Phi}$	energy requirement for non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	g C g N^{-1}	5	(Waring and Running, 1998)
$\boldsymbol{F_h}$	fraction of products from microbial decomposition that are humified (function of clay content)		0.167 + 0.167*clay	
$\boldsymbol{F_l}$	fraction of microbial growth allocated to labile component $M_{i,n,l}$		0.55	(Grant et al., 1993a, b)
$\boldsymbol{F_r}$	fraction of microbial growth allocated to resistant component $M_{i,n,r}$		0.45	(Grant et al., 1993a, b)
F_s	equilibrium ratio between $Q_{i,l,C}$ and $H_{i,l,C}$			
$f_{di,n,l N,P}$	fraction of N or P released with $D_{Mi,n,j,l,C}$ during decomposition	dimensionless	0.33 $U_{NH4} > 0$ 1.00 $U_{NH4} < 0$ 0.33 $U_{PO4} > 0$ 1.00 $U_{PO4} < 0$	
f_{tgl}	temperature function for microbial growth respiration	dimensionless		
f_{tml}	temperature function for maintenance respiration	dimensionless		
$f_{\psi gl}$	soil water potential function for microbial, root or mycorrhizal growth respiration	dimensionless		(Pirt, 1975)
$\Phi_{i,n=f,j,l}$	non-symbiotic N_2 fixation by heterotrophic diazotrophs (n = f)	g N m^{-2} h^{-1}		
$G_{i,l,C}$	total C in substrate-microbe complex	g C Mg^{-1}		
$[H_2PO_4^-]$	concentration of $H_2PO_4^-$ in soil solution	g P m^{-3}		

$\boldsymbol{H}_{\mathbf{a}}$	energy of activation	J mol^{-1}	65 x 10^3	(Addiscott, 1983)
$\boldsymbol{H}_{\mathbf{dh}}$	energy of high temperature deactivation	J mol^{-1}	225 x 10^3	
$\boldsymbol{H}_{\mathbf{dl}}$	energy of low temperature deactivation	J mol^{-1}	198 x 10^3	
$H_{Mi,n,j,l,\mathrm{C}}$	transfer of microbial C decomposition products to humus	g C m m^{-2} h^{-1}		
$H_{Mi,n,j,l,\mathrm{N,P}}$	transfer of microbial N or P decomposition products to humus	g N or P m^{-2} h^{-1}		
$H_{Si,j,l,\mathrm{C}}$	transfer of C hydrolysis products to particulate OM	g C m^{-2} h^{-1}		
$H_{Si,j,l,\mathrm{N,P}}$	transfer of N or P hydrolysis products to particulate OM	g N or P m^{-2} h^{-1}		
$\boldsymbol{K}_{iS}$	inhibition constant for microbial colonization of substrate	-	0.5	(Grant et al., 2010)
$\boldsymbol{K}_{\mathbf{NH_4}}$	M-M constant for NH_4^+ uptake at microbial surfaces	g N m^{-3}	0.40	
$\boldsymbol{K}_{\mathbf{NO_3}}$	M-M constant for NO_3^- uptake at microbial surfaces	g N m^{-3}	0.35	
$\boldsymbol{K}_{\mathbf{PO_4}}$	M-M constant for $H_2PO_4^-$ uptake at microbial surfaces	g P m^{-3}	0.125	
$\boldsymbol{K}_{\mathbf{i}D}$	inhibition constant for $[M_{i,n,a}]$ on $S_{i,\mathrm{C}}$, $Z_{i,\mathrm{C}}$	g C m^{-3}	25	(Lizama and Suzuki, 1991 ; Grant et al., 1993a, b)
$\boldsymbol{K}_{\mathbf{m}D}$	Michaelis–Menten constant for $D_{Si,j,\mathrm{C}}$	g C Mg^{-1}	75	
$\boldsymbol{K}_{\mathbf{m}Q_\mathrm{C}}$	Michaelis–Menten constant for $R'_{\mathrm{h}i,n}$ on $[Q_{i,\mathrm{C}}]$	g C m^{-3}	36	
$\boldsymbol{K}_{\mathbf{O_2}}$	Michaelis–Menten constant for reduction of O_{2s} by microbes, roots and mycorrhizae	g O_2 m^{-3}	0.064	(Griffin, 1972)
$\boldsymbol{k}_{\mathbf{ts}}$	equilibrium rate constant for sorption	h^{-1}	0.01	(Grant et al., 1993a, b)
$\boldsymbol{L}_{\mathbf{h}j}$	ratio of nonlignin to lignin components in humified hydrolysis products		0.10, 0.05, and 0.05 for j = protein, carbohydrate, and cellulose, respectively	(Schulten and Schnitzer, 1997)
$\boldsymbol{M}$	molecular mass of water	g mol^{-1}	18	

$\boldsymbol{M_{i,d,l,C}}$	heterotrophic microbial C used for decomposition	g C m^{-2}	
$M_{i,n,j,l,\mathrm{C}}$	microbial C	g C m^{-2}	
$M_{i,n,j,l,\mathrm{N}}$	microbial N	g N m^{-2}	
$M_{i,n,j,l,\mathrm{P}}$	microbial P	g P m^{-2}	
$M_{i,n,a,l,\mathrm{C}}$	active microbial C from heterotrophic population *n* associated with $G_{i,l,\mathrm{C}}$	g C m^{-2}	
$[M_{i,n,a,l,\mathrm{C}}]$	concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,l,\mathrm{C}} / \theta_l$	g C m^{-3}	
$[NH_4^+{}_{i,n,j,l}]$	concentration of NH_4^+ at microbial surfaces	g N m^{-3}	
$[\mathbf{NH_4^+{}_{mn}}]$	concentration of NH_4^+ at microbial surfaces below which $U_{\mathrm{NH_4}} = 0$	g N m^{-3}	0.0125
$[NO_3^-{}_{i,n,j,l}]$	concentration of NH_4^+ at microbial surfaces	g N m^{-3}	
$[\mathbf{NO_3^-{}_{mn}}]$	concentration of NO_3^- at microbial surfaces below which $U_{\mathrm{NO_3}} = 0$	g N m^{-3}	0.03
$[H_2PO_4^-{}_{i,n,j,l}]$	concentration of $H_2PO_4^-$ at microbial surfaces	g N m^{-3}	
$[\mathbf{H_2PO_4^-{}_{mn}}]$	concentration of $H_2PO_4^-$ at microbial surfaces below which $U_{\mathrm{PO_4}} = 0$	g N m^{-3}	0.002
$[O_{2mi,n,l}]$	O_2 concentration at heterotrophic microsites	g O_2 m^{-3}	
$[O_{2sl}]$	O_2 concentration in soil solution	g O_2 m^{-3}	
$Q_{i,l,\mathrm{C}}$	*DOC* from products of $D_{Si,j,l,\mathrm{C}}$ [SA3] and $D_{Zi,j,l,\mathrm{C}}$ [SA5]	g C m^{-2}	
$[Q_{i,l,\mathrm{C}}]$	solution concentration of $Q_{i,l,\mathrm{C}}$	g C Mg^{-1}	
$Q_{i,l,\mathrm{N,P}}$	*DON* and DOP from products of $(D_{Si,j,l,\mathrm{N,P}} + D_{Zi,j,l,\mathrm{N,P}})$	g N or P m^{-2}	
$\boldsymbol{q_m}$	constant for reallocating $M_{i,a,l,\mathrm{C}}$ to $M_{i,d,l,\mathrm{C}}$	-	0.5

$\boldsymbol{R}$	gas constant	J mol^{-1} K^{-1}	8.3143	
$R_{\Phi i,n=f,j,l}$	respiration for non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	g C m^{-2} h^{-1}		
$R_{\mathrm{g}i,n,l}$	growth respiration of $M_{i,n,a,l}$ on $Q_{i,l,\mathrm{C}}$ under nonlimiting O_2 and nutrients	g C g C^{-1} h^{-1}		
R_{h}	total heterotrophic respiration of all $M_{i,n,a,l}$ under ambient DOC, O_2, nutrients, θ and temperature	g C m^{-2} h^{-1}		
$R_{\mathrm{h}i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under ambient DOC, O_2, nutrients, θ and temperature	g C m^{-2} h^{-1}		
$\boldsymbol{R}_{\mathrm{h}i,n,l}$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2, DOC, θ and 25°C	g C g C^{-1} h^{-1}		
$\boldsymbol{R}_{\mathrm{h}}'{}_{n}$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting DOC, O_2, nutrients, θ and 25°C	g C g C^{-1} h^{-1}	0.125	(Shields et al., 1973)
$R_{\mathrm{h}}'{}_{i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2 and ambient DOC, nutrients, θ and temperature	g C m^{-2} h^{-1}		
$\boldsymbol{R}_{\mathrm{m}}$	specific maintenance respiration at 25°C	g C g N^{-1} h^{-1}	0.0115	(Barnes et al., 1997)
$R_{\mathrm{m}i,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	g C m^{-2} h^{-1}		
$r_{\mathrm{w}l}$	radius of r_{m} + water film at current water content	m		
$\boldsymbol{r}_{\mathbf{m}}$	radius of heterotrophic microsite	m	2.5 × 10^{-6}	
$r_{\mathrm{w}l}$	thickness of water films	m		
$\boldsymbol{S}$	change in entropy	J mol^{-1} K^{-1}	710	(Sharpe and DeMichele, 1977)
$[S_{i,j,l,\mathrm{C}}]$	concentration of $S_{i,j,l,\mathrm{C}}$ in soil	g C Mg^{-1}		
$S_{i,j,l,\mathrm{C}}$	mass of colonized litter, POC or humus C	g C m^{-2}		
$S'_{i,j,l,C}$	mass of uncolonized litter, POC or humus C	g C m^{-2}		

$S_{i,j,l,\mathrm{N,P}}$	mass of litter, POC or humus N or P	g N or P m^{-2}	
T_{sl}	soil temperature	K	
$U_{i,n,l\mathrm{C}}$	uptake of $Q_{i,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g C m^{-2} h^{-1}	
$U_{i,n,\mathrm{N,P}}$	uptake of $Q_{i,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g N or P m^{-2} h^{-1}	
$U_{\mathrm{NH4}i,n,j,l}$	NH_4^+ uptake by microbes	g N m^{-2} h^{-1}	
$\boldsymbol{U'_{\mathrm{NH_4}}}$	maximum $U_{\mathrm{NH_4}}$ at 25 °C and non-limiting NH_4^+	g N m^{-2} h^{-1}	5.0 x 10^{-3}
$U_{\mathrm{NO3}i,n,j,l}$	NO_3^- uptake by microbes	g N m^{-2} h^{-1}	
$\boldsymbol{U'_{\mathrm{NO_3}}}$	maximum $U_{\mathrm{NO_3}}$ at 25 °C and non-limiting NO_3^-	g N m^{-2} h^{-1}	5.0 x 10^{-3}
$U_{\mathrm{O2}i,n}$	O_2 uptake by $M_{i,n,a,l}$ under ambient O_2	g m^{-2} h^{-1}	
$U'_{\mathrm{O2}i,n}$	O_2 uptake by $M_{i,n,a,l}$ under nonlimiting O_2	g m^{-2} h^{-1}	
$U_{\mathrm{PO4}i,n,j,l}$	$H_2PO_4^-$ uptake by microbes	g N m^{-2} h^{-1}	
$\boldsymbol{U'_{\mathrm{PO_4}}}$	maximum $U_{\mathrm{PO_4}}$ at 25 °C and non-limiting $H_2PO_4^-$	g N m^{-2} h^{-1}	5.0 x 10^{-3}
$X_{i,l,\mathrm{C}}$	adsorbed C hydrolysis products	g C Mg^{-1}	
$X_{i,l,\mathrm{N,P}}$	adsorbed N or P hydrolysis products	g P Mg^{-1}	
$\boldsymbol{y}$	selected to give a Q_{10} for f_{tm} of 2.25		0.081
ψ_s	soil or residue water potential	MPa	
$Y_{i,l,\mathrm{C}}$	sorption of C hydrolysis products	g C m^{-2} h^{-1}	
$Y_{i,l,\mathrm{N,P}}$	sorption of N or P hydrolysis products	g P m^{-2} h^{-1}	
$[Z_{i,j,l,\mathrm{C}}]$	concentration of $Z_{i,j,l,\mathrm{C}}$ in soil	g C Mg^{-1}	

$Z_{i,j,l,\mathrm{C}}$	mass of microbial residue C in soil	g C m^{-2}
$Z_{i,j,l,\mathrm{N,P}}$	mass of microbial residue N or P in soil	g P m^{-2}

Appendix B: Soil-plant water relations

Canopy transpiration

$Rn_{ci} + LE_{ci} + H_{ci} + G_{ci} = 0$	canopy energy balance	[SB1a]
$\boldsymbol{L}E_{ci} = L\,(e_{a} - e_{ci(T_{ci},\psi_{ci})})/r_{ai}$	LE from canopy evaporation	[SB1b]
$\boldsymbol{L}E_{ci} = L\,(e_{a} - e_{ci(T_{ci},\psi_{ci})})/(r_{ai} + r_{ci})$ - $\boldsymbol{L}E_{ci}$ [SB1b]	LE from canopy transpiration	[SB1c]
$H_{ci} = \rho C_{p}(T_{a} - T_{ci})/r_{ai}$	H from canopy energy balance	[SB1d]
$r_{cmin\,i} = 0.64\,(C_{b} - \boldsymbol{C_{i}'}_{i})/\,V_{c}'_{i}$	r_{c} driven by rates of carboxylation *vs*. diffusion	[SB2a]
$r_{ci} = r_{cmin\,i} + (\boldsymbol{r_{cmax\,i}} - r_{cmin\,i})\,e^{(-\boldsymbol{\beta}\,\psi_{ti})}$	r_{c} constrained by water status	[SB2b]
$r_{ai} = \{(\ln((z_{u} - z_{di})/z_{ri})^{2}/(\boldsymbol{K}^{2}\,u_{a})\}/(1 - 10\,Ri)$	r_{a} driven by windspeed, surface	[SB3a]
$Ri = \{g\,(z_{u} - z_{ri})/(u_{a}^{2}\,T_{a})\}\,(T_{a} - T_{c})$	r_{a} adjusted for stability *vs.* buoyancy	[SB3b]
$\psi_{ti} = \psi_{ci} - \psi_{\pi i}$		[SB4]

Root/moss/mycorrhizal water uptake

$U_{wi} = \Sigma_{l}\,\Sigma_{r}\,U_{wi,r,l}$		[SB5]
$U_{wi,r,l} = (\psi_{c}'_{i} - \psi_{s}'_{l})/(\Omega_{si,r,l} + \Omega_{ri,r,l} + \Sigma_{x}\,\Omega_{ai,r,l,x})$	U_{w} along hydraulic gradient	[SB6]
$\psi_{c}'_{i} = \psi_{ci} + 0.01\,z_{bi}$		[SB7]
$\psi_{s}'_{l} = \psi_{sl} - 0.01\,z_{l}$		[SB8]
$\Omega_{si,r,l} = \ln\{(d_{i,r,l}/r_{i,r,l})/(2\pi\,L_{i,r,l}\,\kappa_{ri,r,l})\}\;\theta_{wl}/\theta_{pl}$		[SB9]
$\Omega_{ri,r,l} = \boldsymbol{\Omega'_{ri,r}}/L_{i,r,l}$		[SB10]
$\Omega_{ai,r,l,x=1} = \boldsymbol{\Omega'_{ai,r}}\,z_{l}\,/\{n_{i,r,l,1}\,(r_{i,r,l,1}\,/\boldsymbol{r'}_{i,r})^{4}\} + \boldsymbol{\gamma\Omega'_{ai,r}}\,z_{bi}\,/\{n_{i,r,l,1}\,(r_{bi}\,/r_{b}'_{i})^{4}\}\Sigma_{i,r,l}\,(M_{i,r,l})\,/M_{i,r,l}$		[SB11]
$\Omega_{ai,r,l,x=2} = \boldsymbol{\Omega_{ai,r}}\,(L_{i,r,l,2}\,/n_{i,r,l,2})\,/\{n_{i,r,l,2}\,(r_{i,r,l,2}\,/\,r'_{i,r})^{4}\}$		[SB12]
$\delta L_{i,r,l,1}/\delta t = \delta M_{i,r,l,1}\,/\delta t\;\nu_{r}\;/\{\rho_{r}\,(1 - \theta_{Pi,r})\,(\pi\,r_{i,r,l,1}{}^{2})\}$		[SB13]

Canopy water potential

$(e_{a} - e_{i(T_{ci})})/(r_{ai} + r_{ci})$ [SB1] $= \Sigma_{l}\,\Sigma_{r}(\psi_{c}'_{i} - \psi_{s}'_{l})/(\Omega_{si,r,l} + \Omega_{ri,r,l} + \Sigma_{x}\,\Omega_{ai,r,l,x}) + X_{ci}\delta\psi_{ci}/\delta t$	ψ_{c} solved when transpiration from [SB1-SB4] equals uptake from [SB5-SB13] + change in storage	[SB14]

Definition of variables in Appendix B

Variable	Definition	Unit	Equation	Value	Reference
		Subscripts			
I	plant species or functional type: coniferous, deciduous, annual, perennial, C_3, C_4, monocot, dicot etc.				
J	branch or tiller				
K	Node				
L	soil or canopy layer				
M	leaf azimuth				
n	leaf inclination				
o	leaf exposure (sunlit *vs*. shaded)				
r	root/moss/mycorrhizae				
		Variables			
β	stomatal resistance shape parameter	MPa^{-1}	-5.0		(Grant and Flanagan, 2007)
C_b	$[CO_2]$ in canopy air	$\mu mol\ mol^{-1}$			
C'_i	$[CO_2]$ in canopy leaves at $\psi_{c_i} = 0$ MPa	$\mu mol\ mol^{-1}$	0.70 C_b		(Larcher, 2003)
$d_{i,r,l}$	half distance between adjacent roots/mosses	m			
E_{ci}	canopy transpiration	$m^3\ m^{-2}\ h^{-1}$			
e_a	atmospheric vapor density at T_a and ambient humidity	$g\ m^{-3}$			
$e_{ci(T_{ci},\psi_{ci})}$	canopy vapor density at T_{c_i} and ψ_{c_i}	$g\ m^{-3}$			

$G_{\mathbf{c}i}$	canopy storage heat flux	W m^{-2}		
$H_{\mathbf{c}i}$	canopy sensible heat flux	W m^{-2}		
K	von Karman's constant		0.41	
$\kappa_{ri,r,l}$	hydraulic conductivity between soil and root/moss surface	m^2 MPa^{-1} h^{-1}		
γ	scaling factor for bole axial resistance from primary root/moss axial resistance	-	1.6 x 10^4	(Grant et al., 2007)
$\boldsymbol{L}$	latent heat of evaporation	J g^{-1}	2460	
$\boldsymbol{L}E_{ci}$	latent heat flux between canopy and atmosphere	W m^{-2}		
$L_{i,r,l}$	length of roots/mosses/mycorrhizae	m m^{-2}		
$M_{i,r,l}$	mass of roots/mosses/mycorrhizae	g m^{-2}		
$n_{i,r,l,x}$	number of primary (x = 1) or secondary (x = 2) axes	m^{-2}		
$\boldsymbol{\Omega'}_{\mathbf{ai},r}$	axial resistivity to water transport along root/moss/mycorrhizal axes	MPa h m^{-4}	4.0 x 10^9 deciduous 1.0 x 10^{10} coniferous	(Larcher, 2003)
$\Omega_{\mathrm{ai},r,l,x}$	axial resistance to water transport along axes of primary (x = 1) or secondary (x = 2) roots/mosses/mycorrhizae	MPa h m^{-1}		
$\boldsymbol{\Omega'}_{\mathbf{ri},r}$	radial resistivity to water transport from surface to axis of roots/mosses/mycorrhizae	MPa h m^{-2}	1.0 x 10^4	(Doussan et al., 1998)
$\Omega_{\mathrm{ri},r,l}$	radial resistance to water transport from surface to axis of roots/mosses/mycorrhizae	MPa h m^{-1}		
$\Omega_{\mathrm{si},r,l}$	radial resistance to water transport from soil to surface of roots/mosses/mycorrhizae	MPa h m^{-1}		
$\theta_{\mathrm{w}l}$	soil water content	m^3 m^{-3}		

θ_{pl}	soil porosity	m^3 m^{-3}		
$\theta_{p_{i,r}}$	root porosity	m^3 m^{-3}		
Ri	Richarson number			(van Bavel and Hillel, 1976)
Rn_{ci}	canopy net radiation	W m^{-2}		
r_{ai}	aerodynamic resistance to vapor flux from canopy	s m^{-1}		
r_{bi}	radius of bole at ambient ψ_{c_i}	m		
$r_b'_i$	radius of bole at ψ_{c_i} = 0 MPa	m		
r_{ci}	canopy stomatal resistance to vapor flux	s m^{-1}		
$\boldsymbol{r_{cmaxi}}$	canopy cuticular resistance to vapor flux	s m^{-1}	5.0 x 10^3	(Larcher, 2003)
r_{cmini}	minimum r_{c_i} at ψ_{c_i} = 0 MPa	s m^{-1}		
$r_{i,r,l,x}$	radius of primary (x=1) or secondary (x=2) roots/mosses/mycorrhizae at ambient $\psi_{r_{i\,l,z}}$	m		
$\boldsymbol{r'}_{i,r}$	radius of secondary roots/mosses/mycorrhizae at $\psi_{r_{i\,l,z}}$ = 0 MPa	m	2.0 x 10^{-4} tree 1.0 x 10^{-4} bush 0.05 x 10^{-4} mycorrhizae	
ρ_r	root specific density	g C g FW^{-1}	0.05	(Grant, 1998)
T_a	air temperature	K		
T_c	canopy temperature	K		
U_{wi}	total water uptake from all rooted soil layers	m^3 m^{-2} h^{-1}		
$U_{wi,r,l}$	water uptake by root/moss/mycorrhizal surfaces in each soil layer	m^3 m^{-2} h^{-1}		

u_a	wind speed measured at z_u	m s^{-1}		
$V_c{}'_i$	potential canopy CO_2 fixation rate at ψ_{c_i} = 0 MPa	µmol m^{-2} s^{-1}		
ν_r	root specific volume	m^3 g FW^{-1}	10^{-6}	(Grant, 1998)
X_{ci}	canopy capacitance	m^3 m^{-2} MPa^{-1}		
ψ_{ci}	canopy water potential	MPa		
$\psi_c{}'_i$	ψ_{ci} + canopy gravitational potential	MPa		
$\psi_{\pi i}$	canopy osmotic potential	MPa		
ψ_{sl}	soil water potential	MPa		
$\psi_s{}'_l$	ψ_{sl} + soil gravitational potential	MPa		
ψ_{ti}	canopy turgor potential	MPa	1.25 at $\psi_c = 0$	
z_{bi}	length of bole from soil surface to top of canopy	m		
z_{di}	canopy zero-plane displacement height	m		(Perrier, 1982)
z_l	depth of soil layer below surface	m		
z_r	canopy surface roughness	m		(Perrier, 1982)
z_u	height of wind speed measurement	m		

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Appendix C: Gross primary productivity and autotrophic respiration

C_3 gross primary productivity

$GPP = \Sigma_{i,j,k,l,m,n,o} \left(V_{\mathrm{c}i,j,k,l,m,n,o} = V_{\mathrm{g}i,j,k,l,m,n,o}\right) A_{i,j,k,l,m,n,o}$	solve for $C_{\mathrm{i}i,j,k,l,m,n,o}$ at which $V_{\mathrm{c}i,j,k,l,m,n,o} = V_{\mathrm{g}i,j,k,l,m,n,o}$	[SC1]
$V_{\mathrm{g}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - C_{\mathrm{i}i,j,k,l,m,n,o})/r_{\mathrm{l}i,j,k,l,m,n,o}$	diffusion	[SC2]
$V_{\mathrm{c}i,j,k,l,m,n,o} = min\{V_{\mathrm{b}i,j,k,l,m,n,o}, V_{\mathrm{j}i,j,k,l,m,n,o}\}$	carboxylation	[SC3]
$r_{\mathrm{l}i,j,k,l,m,n,o} = r_{\mathrm{lmin}i,j,k,l,m,n,o} + (r_{\mathrm{lmax}i} - r_{\mathrm{lmin}i,j,k,l,m,n,o})\, e^{(-\boldsymbol{\beta}\psi_{\mathrm{t}i})}$	r_{l} is leaf-level equivalent of r_{c}	[SC4]
$r_{\mathrm{lmin}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - \boldsymbol{C_{\mathrm{i}}'_i})/ V_{\mathrm{c}}'_{i,j,k,l,m,n,o}$	minimum r_{l} is driven by carboxylation	[SC5]
$V_{\mathrm{b}i,j,k,l,m,n,o} = V_{\mathrm{bmax}i,j,k}(C_{\mathrm{c}i,j,k,l,m,n,o} - \Gamma_{i,j,k})/(C_{\mathrm{c}i,j,k,l,m,n,o}) + K_{\mathrm{c}_i})\, f_{\psi\, i,j,k,l,m,n,o}\; f_{\mathrm{iC}\boldsymbol{i}}$	CO_2, water, temperature and nutrient constraints on V_{b}	[SC6a]
$V_{\mathrm{bmax}_{i,j,k}} = \boldsymbol{V_{\mathrm{b}}'}_i\, \boldsymbol{F}_{\mathbf{rubisco}_i}\, M_{i,j,k,prot}/A_{i,j,k}\; f_{\mathrm{tb}\boldsymbol{i}}$		[SC6b]
$\Gamma_{i,j,k} = 0.5\; O_{\mathrm{c}}\; V_{\mathrm{omax}_{i,j,k}}\; \boldsymbol{K}_{\mathbf{c}_i}/(V_{\mathrm{bmax}_{i,j,k}}\; \boldsymbol{K}_{\mathbf{o}_i})$		[SC6c]
$V_{\mathrm{omax}_{i,j,k}} = \boldsymbol{V_{\mathrm{o}}'}_i\, \boldsymbol{F}_{\mathbf{rubisco}_i}\, M_{i,j,k,prot}/A_{i,j,k}\; f_{\mathrm{to}\boldsymbol{i}}$		[SC6d]
$K_{\mathrm{c}_i} = \boldsymbol{K}_{\mathbf{c}_i}\, f_{\mathrm{tkc}i}\, (1 + O_{\mathrm{c}}/ (\boldsymbol{K}_{\mathbf{o}_i} f_{\mathrm{tko}i}))$		[SC6e]
$V_{\mathrm{j}i,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o}\, Y_{i,j,k,l,m,n,o}\, f_{\psi\, i,j,k,l,m,n,o}\; f_{\mathrm{iC}\boldsymbol{i}}$	water, temperature and nutrient constraints on V_{j}	[SC7]
$J_{i,j,k,l,m,n,o} = (\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k} - ((\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k})^2 - 4\boldsymbol{\alpha\varepsilon}\, I_{i,l,m,n,o}\, J_{\mathrm{max}i,j,k})^{0.5})/(2\boldsymbol{\alpha})$		[SC8a]
$J_{\mathrm{max}i,j,k} = \boldsymbol{V_{\mathrm{j}}'}_i\, \boldsymbol{F}_{\mathbf{chlorophyll}_i}\, M_{i,j,k,prot}/A_{i,j,k}\; f_{\mathrm{tj}i}$		[SC8b]
$f_{\psi\, i,j,k,l,m,n,o} = (r_{\mathrm{lmin}_{i,j,k,l,m,n,o}} / r_{\mathrm{l}_{i,j,k,l,m,n,o}})^{0.5}$	non-stomatal effect related to stomatal effect	[SC9]

$$f_{\mathrm{tb}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\} \quad \text{[SC10a]}$$

$$f_{\mathrm{to}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{o}} - \boldsymbol{H}_{\mathbf{ao}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]] \quad \text{[SC10b]}$$

$$f_{\mathrm{tj}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{j}} - \boldsymbol{H}_{\mathbf{aj}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\} \quad \text{[SC10c]}$$

$$f_{\mathrm{tkc}i} = \exp[\boldsymbol{B}_{\mathbf{kc}} - \boldsymbol{H}_{\mathbf{akc}}/(\boldsymbol{R}T_{\mathrm{c}i})] \quad \text{[SC10d]}$$

$$f_{\mathrm{tko}i} = \exp[\boldsymbol{B}_{\mathbf{ko}} - \boldsymbol{H}_{\mathbf{ako}}/(\boldsymbol{R}T_{\mathrm{c}i})] \quad \text{[SC10e]}$$

Arrhenius functions for carboxylation, oxygenation and electron transport temperature sensitivity of $\boldsymbol{K}_{\mathbf{c}_i}$, $\boldsymbol{K}_{\mathbf{o}_i}$

$$f_{\mathrm{iC}i} = min\{\sigma_{\mathrm{N}i,j}/(\sigma_{\mathrm{N}i,j} + \sigma_{\mathrm{C}i,j}/\boldsymbol{K}_{\mathbf{iC_N}}),\ \sigma_{\mathrm{P}i,j}/(\sigma_{\mathrm{P}i,j} + \sigma_{\mathrm{C}i,j}/\boldsymbol{K}_{\mathbf{iC_P}})\} \quad \text{[SC11]}$$

product inhibition of V_b, V_j from σ_N and σ_P *vs.* σ_C in shoots

$$\delta M_{\mathrm{L_R}i,j,k}/\delta t = \delta M_{\mathrm{L}_{i,j,k}}/\delta t\ \min\{[\boldsymbol{N'}_{\mathbf{leaf}} + (\boldsymbol{N}_{\mathbf{leaf}} - \boldsymbol{N'}_{\mathbf{leaf}})\, f_{\mathrm{iC}i}]/\mathbf{N}_{\mathbf{prot}},\ [\boldsymbol{P'}_{\mathbf{leaf}} + (\boldsymbol{P}_{\mathbf{leaf}} - \boldsymbol{P'}_{\mathbf{leaf}})\, f_{\mathrm{iC}i}]/\mathrm{P}_{\mathrm{prot}}\} \quad \text{[SC12]}$$

leaf structural protein growth

Autotrophic respiration

$$R_\mathrm{a} = \Sigma_i \Sigma_j (R_{\mathrm{c}i,j} + R_{\mathrm{s}i,j}) + \Sigma_i \Sigma_l \Sigma_z (R_{\mathrm{c}i,r,l} + R_{\mathrm{s}i,r,l}) + \boldsymbol{E}_{\mathbf{N,P}} (U_{\mathrm{NH4}i,r,l} + U_{\mathrm{NO3}i,r,l} + U_{\mathrm{PO4}i,r,l}) \quad \text{[SC13]}$$

total autotrophic respiration

$$R_{\mathrm{c}i,j} = \boldsymbol{R}_\mathrm{c}' \sigma_{\mathrm{C}i,j}\, f_{\mathrm{ta}i} \quad \text{[SC14a]}$$

$$R_{\mathrm{c}i,r,l} = \boldsymbol{R}_\mathrm{c}' \sigma_{\mathrm{C}\ i,r,l}\, f_{\mathrm{ta}\ i,l}\ (U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l}) \quad \text{[SC14b]}$$

$$U_{\mathrm{O2}i,r,l} = U'_{\mathrm{O2}\ i,r,l}\ [\mathrm{O}_{2\mathrm{r}i,r,l}]/([\mathrm{O}_{2\mathrm{r}i,r,l}] + \boldsymbol{K}_{\mathbf{O_2}}) \quad \text{[SC14c]}$$

$$= U_{\mathrm{w}_{i,r,l}} [\mathrm{O}_{2\mathrm{s}l}] + 2\pi L_{i,r,l} D_{\mathrm{sO2}} ([\mathrm{O}_{2\mathrm{s}l}] - [\mathrm{O}_{2\mathrm{r}i,r,l}]) \ln\{(r_{\mathrm{s}l} + r_{\mathrm{r}i,r,l})/r_{\mathrm{r}i,r,l}\} + 2\pi L_{i,r,l} D_{\mathrm{rO2}} ([\mathrm{O}_{2\mathrm{q}i,r,l}] - [\mathrm{O}_{2\ \mathrm{r}i,r,l}]) \ln(r_{\mathrm{q}i,r,l})/r_{\mathrm{r}i,r,l}) \quad \text{[SC14d]}$$

$$U'_{\mathrm{O2}\ i,r,l} = 2.67\, R_\mathrm{a}'{}_{i,r,l} \quad \text{[SC14e]}$$

O_2 constraint on root respiration from active uptake coupled with diffusion of O_2 from soil as for heterotrophic respiration [SA17], and from active uptake coupled with diffusion of O_2 from roots

$$R_{\mathrm{s}i,j} = -\ min\{0.0,\ R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j}\} \quad \text{[SC15]}$$

remobilization when $R_\mathrm{m} > R_\mathrm{c}$

$$R_{\mathrm{m}i,j} = \Sigma_z (\mathrm{N}_{i,j,z}\, \boldsymbol{R}_{\mathbf{m}}'\, f_{\mathrm{tm}i}) \quad \text{[SC16]}$$

maintenance respiration

$$R_{\mathrm{g}i,j} = max\{0.0,\ min\{(R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j})\ min\{1.0,\ max\{0.0,\ \psi_{\mathrm{t}i} - \psi_\mathrm{t}'\}\} \quad \text{[SC17]}$$

growth when $R_\mathrm{m} < R_\mathrm{c}$

Growth and senescence

$$l_{i,j,z,\mathrm{C}} = R_{\mathrm{s}i,j}\, M_{\mathrm{L_N}i,j} / M_{\mathrm{L_R}i,j} \quad \text{[SC18]}$$

senescence drives litterfall of non-remobilizable material

$$l_{i,j,z,\mathrm{N}} = l_{i,j,z,\mathrm{C}}\,\mathbf{N_{prot}}\,(1.0 - \boldsymbol{X}_{\mathbf{mx}}\,f_{\mathrm{xN}i,j}) \quad \text{[SC19a]}$$

$$l_{i,j,z,\mathrm{P}} = l_{i,j,z,\mathrm{C}}\,\mathbf{P_{prot}}\,(1.0 - \boldsymbol{X}_{\mathbf{mx}}\,f_{\mathrm{xP}i,j}) \quad \text{[SC19b]}$$

$$f_{\mathrm{xN}i,j} = \sigma_{\mathrm{C}i,j}/(\sigma_{\mathrm{C}i,j} + \sigma_{\mathrm{N}i,j}/\boldsymbol{K}_{\mathbf{xN}}) \quad \text{[SC19c]}$$

$$f_{\mathrm{xP}i,j} = \sigma_{\mathrm{C}i,j}/(\sigma_{\mathrm{C}i,j} + \sigma_{\mathrm{P}i,j}/\boldsymbol{K}_{\mathbf{xP}}) \quad \text{[SC19d]}$$

litterfall of N and P is driven by that of C but reduced by translocation to to σ_{N} and σ_{P} according to ratios of σ_{N} and σ_{P} with σ_{C}

$$\delta M_{\mathrm{B}i,j}/\delta t = \Sigma_z\,[R_{\mathrm{g}i,j}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,z})/\boldsymbol{Y}_{\mathbf{g}i,z}] - R_{\mathrm{s}i,j} - l_{i,j,\mathrm{C}} \quad \text{[SC20a]}$$

branch growth driven by R_{g}

$$\delta M_{\mathrm{R}i,r,l}/\delta t = [R_{\mathrm{g}i,r,l}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,r})/\boldsymbol{Y}_{\mathbf{g}i,r}] - R_{\mathrm{s}i,r,l} - l_{i,r,l,\mathrm{C}} \quad \text{[SC20b]}$$

root growth driven by R_{g}

$$\delta A_{\mathrm{L}i,j,k,l}/\delta t = \boldsymbol{\chi}\,(M_{\mathrm{L}i,j,k,l}/y_i)^{-0.33}\,\delta M_{\mathrm{L}i,j,k,l}/\delta t\,\min\{1, \max\{0, \psi_{ti} - \psi_t'\} \quad \text{[SC21a]}$$

leaf expansion driven by leaf mass growth

$$\delta L_{i,r,l,1}/\delta t = (\delta M_{\mathrm{R}i,r,l,1}/\delta t)/y_i\,\nu_r/\{\boldsymbol{\rho}_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r})\,(\pi\,r_{\mathrm{r}i,r,l,1}{}^2)\} \quad \text{[SC21b]}$$

$$\delta L_{i,r,l,2}/\delta t = (\delta M_{\mathrm{R}i,r,l,2}/\delta t)\,\nu_r/\{\boldsymbol{\rho}_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r})\,(\pi\,r_{\mathrm{r}i,r,l,2}{}^2)\} \quad \text{[SC21c]}$$

root extension of primary and secondary axes driven by root mass growth

$$f_{\mathrm{ta}i} = T_{\mathrm{c}i}\{\exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}}/(\boldsymbol{R}T_{\mathrm{c}i})]\}/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\} \quad \text{[SC22a]}$$

Arrhenius function for R_{a}

$$f_{\mathrm{tm}i} = e^{(0.0811*(T_{ci} - 298.15))} \quad \text{[SC22b]}$$

temperature function for R_{m}

Root/moss/mycorrhizal nutrient uptake

$$U_{\mathrm{NH4}i,r,l} = \{U_{\mathrm{w}i,r,l}[\mathrm{NH_4^+}{}_l] + 2\pi L_{i,r,l}D_{\mathrm{eNH_4}l}\,([\mathrm{NH_4^+}{}_l] - [\mathrm{NH_4^+}{}_{i,r,l}])\,/\,\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\} \quad \text{[SC23a]}$$

$$= \boldsymbol{U'}_{\mathbf{NH_4}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{NH_4^+}{}_{i,r,l}] - [\mathbf{NH_4^+{}_{mn}}])/([\mathrm{NH_4^+}{}_{i,r,l}] - [\mathbf{NH_4^+{}_{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\,f_{\mathrm{t}il}\,f_{\mathrm{iN}\boldsymbol{i,r,l}} \quad \text{[SC23b]}$$

$$U_{\mathrm{NO3}i,r,l} = \{U_{\mathrm{w}i,r,l}\,[\mathrm{NO_3^-}{}_l] + 2\pi L_{i,r,l}\,D_{\mathrm{eNO_3}l}\,([\mathrm{NO_3^-}{}_l] - [\mathrm{NO_3^-}{}_{i,r,l}])\,/\,\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\} \quad \text{[SC23c]}$$

$$= \boldsymbol{U'}_{\mathbf{NO_3}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{NO_3^-}{}_{i,r,l}] - [\mathbf{NO_3^-{}_{mn}}])/([\mathrm{NO_3^-}{}_{i,r,l}] - [\mathbf{NO_3^-{}_{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\,f_{\mathrm{t}il}\,f_{\mathrm{iN}\boldsymbol{i,r,l}} \quad \text{[SC23d]}$$

$$U_{\mathrm{PO4}i,r,l} = \{U_{\mathrm{w}i,r,l}\,[\mathrm{H_2PO_4^-}{}_l] + 2\pi L_{i,r,l}D_{\mathrm{ePO_4}l}\,([\mathrm{H_2PO_4^-}{}_l] - [\mathrm{H_2PO_4^-}{}_{i,r,l}])\,/\,\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\} \quad \text{[SC23e]}$$

$$= \boldsymbol{U'}_{\mathbf{PO_4}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{H_2PO_4^-}{}_{i,r,l}] - [\mathbf{H_2PO_4^-{}_{mn}}])/([\mathrm{H_2PO_4^-}{}_{i,r,l}] - [\mathbf{H_2PO_4^-{}_{mn}}] + \boldsymbol{K}_{\mathbf{PO_4}})\,f_{\mathrm{t}gl}\,f_{\mathrm{iP}\boldsymbol{i,r,l}} \quad \text{[SC23f]}$$

$$f_{\mathrm{iN}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{N}i,r,l}/\boldsymbol{K}_{\mathbf{iN_C}}) \quad \text{[SC23g]}$$

$$f_{\mathrm{iP}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{P}i,r,l}/\boldsymbol{K}_{\mathbf{iP_C}}) \quad \text{[SC23h]}$$

Root/moss/mycorrhizal N and P uptake from mass flow + diffusion coupled with active uptake of NH_4^+, NO_3^- and $H_2PO_4^-$ constrained by O_2 uptake, as for microbial N and P uptake [SA26]

product inhibition of U_{NH4}, U_{NO3} and U_{PO4} determined by σ_{N} and σ_{P} *vs.* σ_{C} in roots

Definition of variables in Appendix C

Variable	Definition	Unit	Value	Reference
		Subscripts		
i	species or functional type: evergreen, coniferous, deciduous, annual, perennial, C_3, C_4, monocot, dicot, legume etc.			
j	branch or tiller			
k	Node			
l	soil or canopy layer			
m	leaf azimuth			
n	leaf inclination			
o	leaf exposure (sunlit *vs*. shaded)			
z	organ including leaf, stem, root, moss mycorrhizae			
		Variables		
A	leaf, root/moss/mycorrhizal surface area	$m^2\ m^{-2}$		
$\boldsymbol{\beta}$	shape parameter for stomatal effects on CO_2 diffusion and non-stomatal effects on carboxylation	MPa^{-1}	-5.0	(Grant and Flanagan, 2007)
B	parameter such that f_t = 1.0 at T_c = 298.15 K		17.533	
$\boldsymbol{B_j}$	parameter such that $f_{tj\boldsymbol{i}}$ = 1.0 at T_c = 298.15 K		17.363	
$\boldsymbol{B_{kc}}$	parameter such that f_{tkci} = 1.0 at T_c = 298.15 K		22.187	
$\boldsymbol{B_{ko}}$	parameter such that f_{tkoi} = 1.0 at T_c = 298.15 K		8.067	
$\boldsymbol{B_o}$	parameter such that $f_{to\boldsymbol{i}}$ = 1.0 at T_c = 298.15 K		24.221	

$\boldsymbol{B}_v$	parameter such that f_{tvi} = 1.0 at T_c = 298.15 K		26.238	
C_b	[CO_2] in canopy air	μmol mol^{-1}		
$C_{c(b4)}$	[CO_2] in C_4 bundle sheath	μM		
$C_{c(m4)}$	[CO_2] in C_4 mesophyll in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM		
C_c	[CO_2] in canopy chloroplasts in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM		
$C_{i(m4)}'$	[CO_2] in C_4 mesophyll air when ψ_{ci} = 0	μmol mol^{-1}	0.45 x C_b	
$C_{i(m4)}$	[CO_2] in C_4 mesophyll air	μmol mol^{-1}		
$C_{i,j,z=l}$	C content of leaf ($z = l$)	g C m^{-2}		
$\boldsymbol{C}_i'$	[CO_2] in canopy leaves when ψ_{ci} = 0	μmol mol^{-1}	0.70 x C_b	(Larcher, 2003)
C_i	[CO_2] in canopy leaves	μmol mol^{-1}		
$D_{e\ NH_4l}$	effective dispersivity-diffusivity of NH_4^+ during root/moss/mycorrhizal uptake	m^2 h^{-1}		
$D_{e\ NO_3l}$	effective dispersivity-diffusivity of NO_3^- during root/moss/mycorrhizal uptake	m^2 h^{-1}		
$D_{e\ PO_4l}$	effective dispersivity-diffusivity of $H_2PO_4^-$ during root/moss/mycorrhizal uptake	m^2 h^{-1}		
D_{rO2}	aqueous diffusivity of O_2 from root aerenchyma to root or mycorrhizal surfaces	m^2 h^{-1}		
D_{sO2}	aqueous diffusivity of O_2 from soil to root or mycorrhizal surfaces	m^2 h^{-1}		
$d_{i,r,l}$	half distance between adjacent roots assumed equal to uptake path length	m	$(\pi\ L_{s,z}/\Delta z)^{-1/2}$	(Grant, 1998)

$\boldsymbol{E}_{\mathbf{N,P}}$	energy cost of nutrient uptake	g C g N^{-1} or P^{-1}	2.15	(Veen, 1981)
$f_{C(c3)}$	C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll	–		
$f_{C(m4)}$	C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	–		
$\boldsymbol{F}_{\mathbf{chl}}$	fraction of leaf protein in chlorophyll	-	0.025	
f_{iC}	N,P inhibition on carboxylation, leaf structural N,P growth	–		
f_{iN}	N inhibition on root/moss/mycorrhizal N uptake	–		
f_{iP}	P inhibition on root/moss/mycorrhizal P uptake	–		
$\boldsymbol{F}_{\mathbf{rubisco}}$	fraction of leaf protein in rubisco	-	0.125	
f_{ta}	temperature effect on $R_{ai,j}$	–		
f_{tb}	temperature effect on carboxylation	–		
f_{tg}	temperature function for root/moss/mycorrhizal growth respiration	dimensionless		
f_{tj}	temperature effect on electron transport			
f_{tkc}	temperature effect on $\boldsymbol{K}_{\mathbf{c}_i}$			(Bernacchi et al., 2001, 2003)
f_{tko}	temperature effect on $\boldsymbol{K}_{\mathbf{o}_i}$			(Bernacchi et al., 2001, 2003)
f_{tm}	temperature effect on $R_{mi,j}$	–	$Q_{10} = 2.25$	
f_{to}	temperature effect on oxygenation			
f_{tv}	temperature effect on carboxylation	–		

f_{xN}	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ N translocated out of leaf or root/moss during senescence	–		
f_{xP}	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ P translocated out of leaf or root/moss during senescence	–		
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–		(Medrano et al., 2002)
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–		
H_a	energy of activation	J mol^{-1}	57.5 x 10^3	
$\boldsymbol{H}_{\mathbf{aj}}$	energy of activation for electron transport	J mol^{-1}	43 x 10^3	(Bernacchi et al., 2001, 2003)
$\boldsymbol{H}_{\mathbf{akc}}$	parameter for temperature sensitivity of $\boldsymbol{K}_{\mathbf{c}_i}$	J mol^{-1}	55 x 10^3	(Bernacchi et al., 2001, 2003)
$\boldsymbol{H}_{\mathbf{ako}}$	parameter for temperature sensitivity of $\boldsymbol{K}_{\mathbf{o}_i}$	J mol^{-1}	20 x 10^3	(Bernacchi et al., 2001, 2003)
$\boldsymbol{H}_{\mathbf{ao}}$	energy of activation for oxygenation	J mol^{-1}	60 x 10^3	(Bernacchi et al., 2001, 2003)
$\boldsymbol{H}_{\mathbf{av}}$	energy of activation for carboxylation	J mol^{-1}	65 x 10^3	(Bernacchi et al., 2001, 2003)
$\boldsymbol{H}_{\mathbf{dh}}$	energy of high temperature deactivation	J mol^{-1}	222.5 x 10^3	
H_{dh}	energy of high temperature deactivation	J mol^{-1}	220 x 10^3	
$\boldsymbol{H}_{\mathbf{dl}}$	energy of low temperature deactivation	J mol^{-1}	198.0 x 10^3	
H_{dl}	energy of low temperature deactivation	J mol^{-1}	190 x 10^3	
I	Irradiance	μmol m^{-2} s^{-1}		

$J_{(b4)}$	electron transport rate in C_4 bundle sheath	μmol m^{-2} s^{-1}		
$J_{(m4)}$	electron transport rate in C_4 mesophyll	μmol m^{-2} s^{-1}		
J	electron transport rate in C_3 mesophyll	μmol m^{-2} s^{-1}		
J_{max}'	specific electron transport rate at non-limiting I and 25^{o}C when ψ_{ci} = 0 and nutrients are nonlimiting	μmol g^{-1} s^{-1}	400	
$J_{max(b4)}$	electron transport rate in C_4 bundle sheath at non-limiting I	μmol m^{-2} s^{-1}		
$J_{max(m4)}$	electron transport rate in C_4 mesophyll at non-limiting I	μmol m^{-2} s^{-1}		
J_{max}	electron transport rate at non-limiting I, ψ_{ci}, temperature and N,P	μmol m^{-2} s^{-1}		
$K_{c(b4)}$	Michaelis-Menten constant for carboxylation in C_4 bundle sheath	μM	30.0 at 25^{o}C and zero O_2	(Lawlor, 1993)
$K_{c(m4)}$	Michaelis-Menten constant for carboxylation in C_4 mesophyll	μM	3.0 at 25^{o}C	(Lawlor, 1993)
$\boldsymbol{K_c}$	Michaelis-Menten constant for carboxylation at zero O_2	μM	12.5 at 25 ^{o}C	(Farquhar et al., 1980)
K_c	Michaelis-Menten constant for carboxylation at ambient O_2	μM		
$\boldsymbol{K_{iC_N}}$	inhibition constant for growth in shoots from σ_C *vs*. σ_N	g C g N^{-1}	100	(Grant, 1998)
$\boldsymbol{K_{iC_P}}$	inhibition constant for growth in shoots from σ_C *vs*. σ_P	g C g P^{-1}	1000	(Grant, 1998)
$K_{I\chi_{C4(b4)}}$	constant for CO_2 product inhibition of C_4 decarboxylation in C_4 bundle sheath	μM	1000.0	

$K_{I\chi_{C4(m4)}}$	constant for C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	μM	5×10^6	
$K_{I\nu_{lf}}$	constant for C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll caused by $[\nu_{lfi,j}]$	$g\ C\ g\ N^{-1}$	100	
$K_{I\pi_{lf}}$	constant for C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll caused by $[\pi_{lfi,j}]$	$g\ C\ g\ P^{-1}$	1000	
$\boldsymbol{K}_{\mathbf{iN_C}}$	inhibition constant for N uptake in roots/mosses from $\sigma_{Ci,j}$ *vs.* σ_{Nj}	$g\ N\ g\ C^{-1}$	0.1	(Grant, 1998)
$\boldsymbol{K}_{\mathbf{iP_C}}$	inhibition constant for P uptake in roots/mosses from $\sigma_{Ci,j}$ *vs.* $\sigma_{Pi,j}$ roots	$g\ P\ g\ C^{-1}$	0.01	(Grant, 1998)
$\boldsymbol{K}_{\mathbf{NH_4}}$	M-M constant for NH_4^+ uptake at root/moss/mycorrhizal surfaces	$g\ N\ m^{-3}$	0.40	(Barber and Silberbush, 1984)
$\boldsymbol{K}_{\mathbf{NO_3}}$	M-M constant for NO_3^- uptake at root/moss/mycorrhizal surfaces	$g\ N\ m^{-3}$	0.35	(Barber and Silberbush, 1984)
$\boldsymbol{K}_{\mathbf{PO_4}}$	M-M constant for $H_2PO_4^-$ uptake root/moss/mycorrhizal surfaces	$g\ P\ m^{-3}$	0.125	(Barber and Silberbush, 1984)
$\boldsymbol{K}_{\mathbf{O_2}}$	Michaelis-Menten constant for root or mycorrhizal O_2 uptake	$g\ m^{-3}$	0.064	(Griffin, 1972)
$\boldsymbol{K}_{\mathbf{o}}$	inhibition constant for O_2 in carboxylation	μM	500 at 25 ºC	(Farquhar et al., 1980)
$\boldsymbol{K}_{\mathbf{xN}}$	inhibition constant for remobilization of leaf or root/moss N during senescence	$g\ N\ g\ C^{-1}$	0.1	
$\boldsymbol{K}_{\mathbf{xP}}$	inhibition constant for remobilization of leaf or root/moss P during senescence	$g\ P\ g\ C^{-1}$	0.01	
L	root length	$m\ m^{-2}$		

l_C	C litterfall from leaf or root/moss	g C m^{-2} h^{-1}		
$l_{N,P}$	N or P litterfall from leaf or root/moss	g C m^{-2} h^{-1}		
M_B	branch C phytomass	g C m^{-2}		
M_L	leaf C phytomass	g C m^{-2}		
M_{L_N}, M_{L_R}	non-remobilizable, remobilizable leaf C phytomass	g C m^{-2}		
M_R	root C phytomass	g C m^{-2}		
M_{iprot}	leaf protein phytomass calculated from leaf N, P contents	g N m^{-2}		
N,P	N or P content of organ z	g N m^{-2}		
$\mathbf{N_{prot}}$	N content of protein remobilized from leaf or root	g N C^{-1}	0.4	
$[NH_4^+{}_{i,r,l}]$	concentration of NH_4^+ at root/moss/mycorrhizal surfaces	g N m^{-3}		
$[\mathbf{NH_4^+{}_{mn}}]$	concentration of NH_4^+ at root/moss/mycorrhizal surfaces below which $U_{NH_4} = 0$	g N m^{-3}	0.0125	(Barber and Silberbush, 1984)
$[NO_3^-{}_{i,r,l}]$	concentration of NH_4^+ at root/moss/mycorrhizal surfaces	g N m^{-3}		
$[\mathbf{NO_3^-{}_{mn}}]$	concentration of NO_3^- at root/moss/mycorrhizal surfaces below which $U_{NO_3} = 0$	g N m^{-3}	0.03	(Barber and Silberbush, 1984)
$[H_2PO_4^-{}_{i,r,l}]$	concentration of $H_2PO_4^-$ root/moss/mycorrhizal surfaces	g N m^{-3}		
$[\mathbf{H_2PO_4^-{}_{mn}}]$	concentration of $H_2PO_4^-$ at root/moss/mycorrhizal surfaces below which $U_{PO_4} = 0$	g N m^{-3}	0.002	(Barber and Silberbush, 1984)
$\boldsymbol{N_{leaf}}$	maximum leaf structural N content	g N g C^{-1}	0.10	
$\boldsymbol{N'_{leaf}}$	minimum leaf structural N content	g N g C^{-1}	0.33 x $\boldsymbol{N_{leaf}}$	
N_{lf}	total leaf N	g N m^{-2} leaf		

$[N_{chl(b4)}]'$	ratio of chlorophyll N in C_4 bundle sheath to total leaf N	g N g N^{-1}	0.05
$[N_{chl(m4)}]'$	ratio of chlorophyll N in C_4 mesophyll to total leaf N	g N g N^{-1}	0.05
$[N_{pep(m4)}]'$	ratio of PEP carboxylase N in C_4 mesophyll to total leaf N	g N g N^{-1}	0.025
$[N_{rub(b4)}]'$	ratio of RuBP carboxylase N in C_4 bundle sheath to total leaf N	g N g N^{-1}	0.025
O_{2q}	aqueous O_2 concentration in root or mycorrhizal aerenchyma	g m^{-3}	
O_{2r}	aqueous O_2 concentration at root or mycorrhizal surfaces	g m^{-3}	
O_{2s}	aqueous O_2 concentration in soil solution	g m^{-3}	
O_c	[O_2] in canopy chloroplasts in equilibrium with O_2 in atm.	μM	
$\boldsymbol{P}_{leaf}$	maximum leaf structural P content	g P g C^{-1}	0.10
$\boldsymbol{P'}_{leaf}$	minimum leaf structural P content	g P g C^{-1}	0.33 x $\boldsymbol{P}_{leaf}$
$\mathbf{P_{prot}}$	P content of protein remobilized from leaf or root	g P C^{-1}	0.04
$[\pi_{lf}]$	concentration of nonstructural root P uptake product in leaf	g P g C^{-1}	
θ_P	root or mycorrhizal porosity	m^3 m^{-3}	0.1 – 0.5
$\boldsymbol{R}$	gas constant	J mol^{-1} K^{-1}	8.3143
R	gas constant	J mol^{-1} K^{-1}	8.3143
R_a	total autotrophic respiration	g C m^{-2} h^{-1}	
R_a'	R_a under nonlimiting O_2	g C m^{-2} h^{-1}	
$\boldsymbol{R}_c'$	specific autotrophic respiration of $\sigma_{Ci,j}$ at T_{ci} = 25 °C	g C g C^{-1} h^{-1}	0.015

R_c	autotrophic respiration of $\sigma_{Ci,j}$ or $\sigma_{Ci,r,l}$	g C m^{-2} h^{-1}		
R_g	growth respiration	g C m^{-2} h^{-1}		
r_{lf}	leaf stomatal resistance	s m^{-1}		
r_{lfmaxi}	leaf cuticular resistance	s m^{-1}		
$r_{lfmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	s m^{-1}		
$r_{li,j,k,l,m,n,o}$	leaf stomatal resistance	s m^{-1}		
r_{lmaxi}	leaf cuticular resistance	s m^{-1}		
$r_{lmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	s m^{-1}		
$\boldsymbol{R_m'}$	specific maintenance respiration of $\sigma_{Ci,j}$ at $T_{ci} = 25$ °C	g C g N^{-1} h^{-1}	0.0115	(Barnes et al., 1997)
$R_{mi,j}$	above-ground maintenance respiration	g C m^{-2} h^{-1}		
$r_{qi,r,l}$	radius of root aerenchyma	m		
$r_{ri,r,l}$	root/moss/mycorrhizal radius	m	1.0×10^{-4} or 5.0×10^{-6}	
$R_{si,j}$	respiration from remobilization of leaf C	g C m^{-2} h^{-1}		
r_{sl}	thickness of soil water films	m		
ρ_r	dry matter content of root/moss biomass	g g^{-1}	0.125	
$\boldsymbol{S}$	change in entropy	J mol^{-1} K^{-1}	710	(Sharpe and DeMichele, 1977)
S	change in entropy	J mol^{-1} K^{-1}	710	
σ_C	nonstructural C product of CO_2 fixation	g C g C^{-1}		

σ_N	nonstructural N product of root/moss/mycorrhizal uptake	$g\ N\ g\ C^{-1}$		
σ_P	nonstructural P product of root/moss/mycorrhizal uptake	$g\ P\ g\ C^{-1}$		
T_c	canopy temperature	K		
T_c	canopy temperature	^oC		
$U_{NH4\,i,r,l}$	NH_4^+ uptake by roots/mosses/mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$		
$\boldsymbol{U'_{NH_4}}$	maximum U_{NH_4} at 25 ^oC and non-limiting NH_4^+	$g\ N\ m^{-2}\ h^{-1}$	5.0 x 10^{-3}	(Barber and Silberbush, 1984)
$U_{NO3\,i,r,l}$	NO_3^- uptake by roots/mosses/mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$		
$\boldsymbol{U'_{NO_3}}$	maximum U_{NO_3} at 25 ^oC and non-limiting NO_3^-	$g\ N\ m^{-2}\ h^{-1}$	5.0 x 10^{-3}	(Barber and Silberbush, 1984)
$U_{PO4\,i,r,l}$	$H_2PO_4^-$ uptake by roots/mosses/mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$		
$\boldsymbol{U'_{PO_4}}$	maximum U_{PO_4} at 25 ^oC and non-limiting $H_2PO_4^-$	$g\ N\ m^{-2}\ h^{-1}$	5.0 x 10^{-3}	(Barber and Silberbush, 1984)
$U_{O2\,i,r,l}$	O_2 uptake by roots and mycorrhizae under ambient O_2	$g\ O\ m^{-2}\ h^{-1}$		
$U'_{O2\,i,l,r}$	O_2 uptake by roots and mycorrhizae under nonlimiting O_2	$g\ O\ m^{-2}\ h^{-1}$		
$U_{w\,i,r,l}$	root/moss/mycorrhizal water uptake	$m^3\ m^{-2}\ h^{-1}$		
$V_{\phi(b4)i,j,k}$	CO_2 leakage from C_4 bundle sheath to C_4 mesophyll	$g\ C\ m^{-2}\ h^{-1}$		
$\boldsymbol{V_b'}$	specific rubisco carboxylation at 25 ^oC	$\mu mol\ g^{-1}$ rubisco s^{-1}	45	(Farquhar et al., 1980)
$V_{b(b4)i,j,k}$	CO_2-limited carboxylation rate in C_4 bundle sheath	$\mu mol\ m^{-2}\ s^{-1}$		
$V_{b(m4)i,j,k,l,m,n,o}$	CO_2-limited carboxylation rate in C_4 mesophyll	$\mu mol\ m^{-2}\ s^{-1}$		

$V_{bi,j,k,l,m,n,o}$	CO_2-limited leaf carboxylation rate	μmol m^{-2} s^{-1}		
$V_{bmax(b4)}'$	RuBP carboxylase specific activity in C_4 bundle sheath at 25°C when ψ_{ci} = 0 and nutrients are nonlimiting	μmol g^{-1} s^{-1}	75	
$V_{bmax(b4)i,j,k}$	CO_2-nonlimited carboxylation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}		
$V_{bmax(m4)}'$	PEP carboxylase specific activity in C_4 mesophyll at 25°C when ψ_{ci} = 0 and nutrients are nonlimiting	μmol g^{-1} s^{-1}	150	
$V_{bmax(m4)i,j,k}$	CO_2-nonlimited carboxylation rate in C_4 mesophyll	μmol m^{-2} s^{-1}		
$V_{bmax i,j,k}$	leaf carboxylation rate at non-limiting CO_2, ψ_{ci}, T_c and N,P	μmol m^{-2} s^{-1}		
$V_{c(b4)i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}		
$V_{c(m4)i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 mesophyll	μmol m^{-2} s^{-1}		
$V_{c0(m4)\,i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 mesophyll when ψ_{ci} = 0 MPa	μmol m^{-2} s^{-1}		
$V_{ci,j,k,l,m,n,o}$	leaf CO_2 fixation rate	μmol m^{-2} s^{-1}		
$V_c'{}_{i,j,k,l,m,n,o}$	leaf CO_2 fixation rate when ψ_{ci} = 0	μmol m^{-2} s^{-1}		
$V_{g(m4)i,j,k,l,m,n,o}$	CO_2 diffusion rate into C_4 mesophyll	μmol m^{-2} s^{-1}		
$V_{gi,j,k,l,m,n,o}$	leaf CO_2 diffusion rate	μmol m^{-2} s^{-1}		
$\boldsymbol{V_j'}$	specific chlorophyll e^- transfer at 25 °C	μmol g $^{-1}$ chlorophyll s^{-1}	450	(Farquhar et al., 1980)
$V_{j(b4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}		

$V_{j(m4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C_4 mesophyll	μmol m^{-2} s^{-1}		
$V_{ji,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	μmol m^{-2} s^{-1}		
$\boldsymbol{V_o'}$	specific rubisco oxygenation at 25 °C	μmol g^{-1} rubisco s^{-1}	9.5	(Farquhar et al., 1980)
$V_{omax i,j,k}$	leaf oxygenation rate at non-limiting O_2, ψ_{ci}, T_c and N,P	μmol m^{-2} s^{-1}		
$V_{\chi C4(b4)i,j,k}$	decarboxylation of C_4 fixation product in C_4 bundle sheath	g C m^{-2} h^{-1}		
$V_{\chi C4(m4)}$	transfer of C_4 fixation product between C_4 mesophyll and bundle sheath	g C m^{-2} h^{-1}		
$[\nu_f]$	concentration of nonstructural root/moss/mycorrhizal N uptake product in leaf	g N g C^{-1}		
ν_r	specific volume of root biomass	m^3 g^{-1}		
$W_{lf(b4)}$	C_4 bundle sheath water content	g m^{-2}		
$W_{lf(m4)}$	C_4 mesophyll water content	g m^{-2}		
X_{mx}	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	0.6	(Kimmins, 2004)
$Y_{(b4)}$	carboxylation yield from electron transport in C_4 bundle sheath	μmol CO_2 μmol e^{-} $^{-1}$		
$Y_{(m4)}$	carboxylation yield from electron transport in C_4 mesophyll	μmol CO_2 μmol e^{-} $^{-1}$		
$\boldsymbol{Y_g}$	fraction of $\sigma_{Ci,j}$ used for growth expended as $R_{gi,j,z}$ by organ z	g C g C^{-1}	0.28 (z = leaf), 0.24 (z = root and other non-foliar), 0.20 (z = wood)	(Waring and Running, 1998)

y	plant population	m^{-2}		
Y	carboxylation yield	μmol CO_2 μmol $e^{-\,-1}$		
Γ	CO_2 compensation point	μM		
$\Gamma_{(b4)}$	CO_2 compensation point in C_4 bundle sheath	μM		
$\Gamma_{(m4)}$	CO_2 compensation point in C_4 mesophyll	μM		
α	shape parameter for response of J to I	-	0.7	
α	shape parameter for response of J to I	-	0.75	
χ	area:mass ratio of leaf growth	m g^{-3}	0.0125	(Grant and Hesketh, 1992)
$\chi_{C4(b4)}$	non-structural C_4 fixation product in C_4 bundle sheath	g C m^{-2}		
$\chi_{C4(m4)}$	non-structural C_4 fixation product in C_4 mesophyll	g C m^{-2}		
$[\chi_{c3(b4)}]$	concentration of non-structural C_3 fixation product in C_4 bundle sheath	g g^{-1}		
$[\chi_{C4(m4)}]$	concentration of non-structural C_4 fixation product in C_4 mesophyll	μM		
ε	quantum yield	μmol e^- μmol $quanta^{-1}$	0.45	(Farquhar et al., 1980)
ε	quantum yield	μmol e^- μmol $quanta^{-1}$	0.45	(Farquhar et al., 1980)
$\kappa_{Cc(b4)}$	conductance to CO_2 leakage from C_4 bundle sheath	h^{-1}	20	
ψ_t	canopy turgor potential	MPa	1.25 at $\psi_c = 0$	

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Appendix D: Soil water, heat and gas fluxes

Surface water flux

$$\frac{\Delta(d_w A)}{\Delta t} = \sum_i Q_{w,in_i} + \sum_i Q_{w,out_i} + P - E_{res} - E_{surf}$$ **;** kinematic wave theory of overland flow [SD1]

$$Q_{w_i} = v_i\left(d_w - d_{sw}\right)L_i \quad \text{[SD2]}$$

$$v_i = \frac{R^{0.67} S_i^{0.5}}{z_r} \quad \text{[SD3]}$$

$$R = \frac{s_r d_{mw}}{s_r^2 + 1} \quad \text{[SD4]}$$

$$S_i = \frac{2abs[\left(Z + d_{sw} + d_{mw}\right)_{s_i} - \left(Z + d_{sw} + d_{mw}\right)_{d_i}]}{L_{s_i} + L_{d_i}} \quad \text{[SD5]}$$

$$E_{res} = \frac{e_{air} - e_{res}(\psi_{res} T_{res})}{r_{a_{res}} + r_{s_{res}}} \quad \text{[SD6]}$$

$$E_{surf} = \frac{e_{air} - e_{surf}(\psi_{surf} T_{surf})}{r_{a_{surf}} + r_{s_{surf}}} \quad \text{[SD7]}$$

Where, subscripts i=dimensions (i=x, y), s=source cell, d=destination cell, in=flow into the grid cells, and out=flow out of the grid cells; d_w=depth of surface water (m); A=area of landscape position (m^2); t=time (h); Q_w=surface water flux (m^3 m^{-2} h^{-1}); P=precipitation flux (m^3 m^{-2} h^{-1}); E_{res}=evaporation flux from surface residue (m^3 m^{-2} h^{-1}); E_{surf}=evaporation flux from soil surface (m^3 m^{-2} h^{-1}); v=velocity of surface water flow (m h^{-1}); ; d_{sw}= maximum depth of surface water storage (m); L=length of grid cells (m); R=ratio of cross-sectional area to perimeter of surface flow (m); S=slope (m m^{-1}); z_r=Manning's roughness coefficient (=0.01 m$^{-1/3}$ h); s_r=slope of channel sides during surface flow (m m^{-1}); Z=surface elevation (m); d_{sw}= maximum depth of surface water storage (m); d_{mw}=depth of mobile surface water (m); e_{air}=atmospheric vapour density (g m^{-3}); e_{res}=vapour density at surface residue (g m^{-3}) at current residue water potential (ψ_{res}) and temperature (T_{res}); $r_{a_{res}}$ =boundary layer resistance to evaporation from surface residue (h m^{-1}); $r_{s_{res}}$ =surface resistance to evaporation from surface residue (h m^{-1}); e_{surf}=vapour density at soil surface (g m^{-3}) at current soil surface water potential (ψ_{surf}) and temperature (T_{surf}); $r_{a_{surf}}$ =boundary layer resistance to evaporation from soil surface (h m^{-1}); and $r_{s_{surf}}$ =surface resistance to evaporation from soil surface (h m^{-1}).

Sub-surface water flux

$$\frac{\Delta\theta_w}{\Delta t} = \sum_i (Q_{w_{mat,in\ i}} + Q_{w_{mac,in\ i}} - Q_{w_{mat,out\ i}} - Q_{w_{mac,out\ i}}) + \sum_j \left(Q_{w_{b,mat,in\ j}} + Q_{w_{b,mac,in\ j}} - Q_{w_{b,mat,out\ j}} - Q_{w_{b,mac,out\ j}}\right) + Q_f - U_w$$; 3D continuity equation for water balance of each soil layer [SD8]

$$Q_{w_{mat\ i}} = K'_{mat_i}(\psi_{s_s} - \psi_{s_d})$$; soil matrix water flow [SD9]

$$K'_{mat_i} = \frac{2K_{mat_{s\ i}} K_{mat_{d\ i}}}{K_{mat_{s\ i}} L_{d\ i} + K_{mat_{d\ i}} L_{s\ i}}$$; when both the source and destination grid cells are either saturated or unsaturated (Richard’s equation) [SD10]

$$K'_{mat_i} = \frac{2K_{mat_{s\ i}}}{L_{s_i} + L_{d_i}}$$; when the source cell is saturated and the destination cell is unsaturated (Green-Ampt equation) [SD11]

$$K'_{mat_i} = \frac{2K_{mat_{d\ i}}}{L_{s_i} + L_{d_i}}$$; when the source cell is unsaturated and the destination cell is saturated (Green-Ampt equation) [SD12]

$$K_{mat_i} = K_{s,mat}\left(\frac{q-p+1}{q}\right)^{1.33}\left[\frac{\sum_{p=1}^{p=q}\frac{2p-1}{\psi_p^2}}{\sum_{r=p}^{r=q}\frac{2r+1-2p}{\psi_r^2}}\right]$$; Green and Corey (1971) model used in MCM simulation of *ecosys* [SD13]

$$p = \mathrm{Int}\left[q\frac{(\theta_s - \theta_p)}{\theta_s}\right] + 1$$ [SD14]

$$n(k) = 1 + 0.001k \quad \text{[SD15]}$$

$$m(k) = 1 - \frac{1}{n(k)} \quad \text{[SD16]}$$

$$\alpha(k) = \frac{m(k)^{1-m(k)}}{\psi_{in}} \quad \text{(van Genuchten 1978)} \quad \text{[SD17]}$$

$$S_{e_{fc,sim}}(k) = \left[1 + (\alpha(k)\psi_{fc})^{n(k)}\right]^{-m(k)} \quad \text{(van Genuchten 1980)} \quad \text{[SD18]}$$

$$S_{e_{wp,sim}}(k) = \left[1 + (\alpha(k)\psi_{wp})^{n(k)}\right]^{-m(k)} \quad \text{(van Genuchten 1980)} \quad \text{[SD19]}$$

$$\theta_r(k) = \max\left[0, \frac{\theta_s - \theta_{v,fc} + \theta_{v,wp}}{S_{e_{fc,sim}}(k) - S_{e_{wp,sim}}(k)}\right] \quad \text{[SD20]}$$

$$\theta_{v,fc_{sim}}(k) = \theta_r(k) + \left[\theta_s - \theta_r(k)\right] S_{e_{fc,sim}}(k) \quad \text{(van Genuchten 1980)} \quad \text{[SD21]}$$

$$\theta_{v,fc_{sim}}(k) = \theta_r(k) + \left[\theta_s - \theta_r(k)\right] S_{e_{fc,sim}}(k) \quad \text{(van Genuchten 1980)} \quad \text{[SD22]}$$

$$K_{mat_i} = K_{s,mat} S_e^{0.5} \left[1 - \left(1 - S_e^{\frac{1}{m}}\right)^m\right]^2 ; \text{where } S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[1 + \left(\alpha\psi_m\right)^n\right]^{-m}$$

; Mualem-van Genuchten model (Mualem, 1976; van Genuchten, 1980) used in VGM simulation of *ecosys* (Mezbahuddin et al., 2016) [SD23]

$$K_{mat_i} = K_{s,mat} S_e^{0.5} \left[\frac{1 - \left(1 - (S_e S_c)^{\frac{1}{m}}\right)^m}{1 - \left(1 - S_c^{\frac{1}{m}}\right)^m}\right]^2 ; \text{where } S_e = \frac{1}{S_c}[1 + (\alpha\psi_m)^n]^{-m} \text{ and } S_c = [1 + (\alpha\psi_e)^n]^{-m}$$

; modified Mualem-van Genuchten model (Ippisch et al., 2006) used in VGM simulation of *ecosys* (Mezbahuddin et al., 2016) [SD24]

$$Q_{w_{mac\ i}} = K'_{mac_i}(\psi_{g_s} - \psi_{g_d})$$; soil macropore water flow [SD25]

$$K'_{mac} = \frac{2K_{mac_s}K_{mac_d}}{K_{mac_s}L_{d_i} + K_{mac_d}L_{s_i}}$$ [SD26]

$$K_{mac} = N_{mac}K^*_{mac}$$ [SD27]

$$K^*_{mac} = \frac{\pi R^4}{8\eta}$$; Hagen-Poiseuille's theory of laminar flow in tubes [SD28]

$$N_{mac} = \theta_{mac}\pi R^2$$ [SD29]

$$Q_{w_{b,mat\ j}} = \frac{K_{b,mat\ j}\left[\psi'_b - \psi_{s_b} + 0.01\left(d_{z_b} - WTD_x\right)\right]}{L_{t_j}}$$; lateral discharge occurs when $d_{z_b} < WTD_x$ and $\psi_{s_b} > \psi'_b + 0.01\left(d_{z_b} - WTD_x\right)$ and lateral recharge occurs when $d_{z_b} > WTD_x$ [SD30]

$$Q_{w_{b,mac\ j}} = \frac{K_{b,mac\ j}\,0.01\left[d_{z_b} - L_{z_b}\left(\theta_{w,mac} - 0.5\right) - WTD_x\right]}{L_{t_j}}$$; lateral discharge occurs when $d_{z_b} < WTD_x$ and lateral recharge occurs when $d_{z_b} > WTD_x$ [SD31]

Where, subscripts *i*=dimensions (*i*=*x*, *y, z*), *j*=dimensions (*j*=*x*, *y*), *s*=source cell, *d*=destination cell, *in*=flow into the grid cells, and *out*=flow out of the grid cells; *b*=boundary grid cell; *mat*=soil matrix/micropore; *mac*=soil macropore; θ_w=soil water content (m^3 m^{-3}); Q_w=sub-surface water flux (m^3 m^{-2} h^{-1}); Q_f=freeze-thaw flux (a positive flux represents thaw and a negative flux represents freeze) (m^3 m^{-2} h^{-1}); U_w=total root water uptake flux (m^3 m^{-2} h^{-1}); K'=hydraulic conductance (m MPa^{-1} h^{-1}); ψ_s=total soil water potential (MPa); *K*=hydraulic conductivity (m^2 MPa^{-1} h^{-1}); *L*=length of the grid cells (m); $K_{s,mat}$=saturated soil matrix hydraulic conductivity (m^2 MPa^{-1} h^{-1}); *p*=individual pore class [1,2,3,…..*q*; where *q*=total number of pore classes (=100)]; ψ_p=matric potential of pore class *p*; ψ_p=matric potential of pore class *r* (*r*=*p*→*q*); *n* =van Genuchten parameter that describes the mean slope of the desorption curve or the range of pore size distribution; α= the inverse of the pressure head at the air-entry value (i.e. $\alpha \approx 1$/air entry potential) that governs the shape of van Genuchten desorption curve (-MPa^{-1}); *k*=number of iteration (1,2,3…..19000); ψ_{in}=matric potential at inflection point (-MPa); $S_{e_{fc,sim}}$ = simulated relative degree of saturation at field capacity; ψ_{fc}=matric potential at field capacity (-MPa); $S_{e_{wp,sim}}$ = simulated relative degree of saturation at wilting point; ψ_{wp}=matric potential at wilting point (-MPa); θ_r =residual soil water content (m^3 m^{-3}); θ_s =soil water content at saturation (m^3 m^{-3}); $\theta_{v,fc}$ =observed input for soil water content at field capacity (m^3 m^{-3}); $\theta_{v,wp}$ =observed input for soil water content at wilting point (m^3 m^{-3}); $\theta_{v,fc_{sim}}$ =simulated soil water content at field capacity (m^3 m^{-3}); $\theta_{v,wp_{sim}}$ =simulated soil water content at wilting point (m^3 m^{-3}); θ=ambient soil water content (m^3 m^{-3}); ψ_m=matric potential as a function of θ (-MPa); ψ_e=matric potential very close to saturation (=-0.0001 MPa); ψ_g=gravitational soil water potential (MPa); N_{mac}=number of macropore channels (m^{-2}); K^*_{mac}=individual macropore hydraulic conductivity (m^4 MPa^{-1} h^{-1} macropore channel^{-1}); η=dynamic viscosity of water (MPa h); θ_{mac}=volumetric macropore fraction (m^3 m^{-3}); R=radius of a macropore channel (m); ψ'=soil water potential at saturation (MPa) (=0 and -0.0005 MPa for van Genuchten and modified Campbell model respectively); d_z=depth of the mid-point of a grid cell from the surface (m); L_z=vertical thickness of a grid cell (m); WTD_x=depth of the water table depth at the adjacent watershed with which modeled grid cells exchange water laterally (m); and L_t=lateral distance over which lateral discharge/recharge occurs (m), MCM = modified Campbell model, VGM = van Genuchten model.

Water table depth

$WTD = -[d_{z,sat} - L_{z,sat}(1 - \frac{\theta_g}{\theta_g^*})]$; negative sign represents depth below the surface of the a particular grid cell [SD32]

Where, WTD=water table depth (m); $d_{z,sat}$=depth to the bottom of the layer immediately above the uppermost saturated layer (m); $L_{z,sat}$=vertical thickness of the layer immediately above the uppermost saturated layer (m); θ_g=current air-filled porosity of the layer immediately above the uppermost saturated layer (m^3 m^{-3}); and θ_g^*=air-filled porosity at air-entry potential of the layer immediately above the uppermost saturated layer (m^3 m^{-3}).

Heat flux

$R_n + LE + H + G = 0$; energy balance for each of the canopy, snow, residue and soil surface [SD33]

$\sum G_{c,in_i} - \sum G_{c,out_i} + L_v Q_f + c(T - T_{frz}) = 0$; 3D general heat flux equation in snowpack, surface residue and soil layers [SD34]

$$T_{frz} = \frac{-9.095895 \times 10^4}{\psi_m - 333} \text{(for residue layer)} = \frac{-9.095895 \times 10^4}{\psi_m + \psi_o - 333} \text{(for soil layers)} = T'_{frz} \text{(for snowpack)} \quad \text{[SD35]}$$

$$G_{c_i} = \frac{2\kappa_{s,d_i}(T_s - T_d)}{L_{s_i} + L_{d_i}} + c_{w_s} T_s Q_{w_i} \quad \text{[SD36]}$$

$$D_{snowpack} = \frac{V_{sweq}\frac{\rho_w}{\rho_{oldsnow}} + V_{ice} + V_{water}}{A_{snowpack}} \quad \text{[SD37]}$$

$$\rho_{oldsnow} = \min(0.5, \rho_{freshsnow} + 0.25\frac{V_{snow}}{A_{snowpack}}) \quad \text{[SD38]}$$

Where, subscripts i=dimensions (i=x, y, z), s=source cell, d=destination cell, in=flow into the grid cells, and out=flow out of the grid cells; R_n=net radiation (Wm^{-2}); LE=latent heat flux (Wm^{-2}); H=sensible heat flux (Wm^{-2}); and G=ground heat flux (Wm^{-2}); G_c=conductive heat flux (MJ m^{-2} h^{-1}); L_v=latent heat of evaporation (=2460 MJ m^{-3}); Q_f=freeze-thaw flux (a positive flux represents thaw and a negative flux represents freeze) (m^3 m^{-2} h^{-1}); c=heat capacity of residue/soil layers (solid + liquid + void) or the snowpack (snow + ice + water) (MJ m^{-2} K^{-1}); T=ambient temperature of soil/residue layers or the snowpack (K); T_{frz}=freezing temperature of soil/residue layers or the snowpack (K); ψ_m=matric water potential of residue/soil layers (-MPa); ψ_o=osmotic potential of soil layers (-MPa); T'_{frz} =freezing temperature of free water (=273.15 K); κ=thermal conductivity (MJ m^{-1} h^{-1} K^{-1}); L=length of the residue layer/ a soil layer/ the snowpack (m); c_w=heat capacity of water (=4.19 MJ m^{-2} K^{-1}) ; Q_w=water flux (m^3 m^{-2} h^{-1}); $D_{snowpack}$=depth of snowpack (m); V_{sweq}=volume of snow water equivalent (m^3); ρ_w=density of water (=1 Mg m^{-3}); $\rho_{oldsnow}$=density of settled snow (Mg m^{-3}); V_{ice}=volume of ice in snowpack (m^3 m^{-3}); V_{water}=volume of water in snowpack (m^3 m^{-3}); $A_{snowpack}$=snowpack basal area (m^2); $\rho_{freshsnow}$=density of freshly fallen snow (=0.083 Mg m^{-3}); V_{snow}=volume of snow in the snowpack (m^3)

Gas flux

$Q_{ds\gamma_s} = \alpha_{gs_s} D_{d\gamma}\left(S'_\gamma f_{T_{d\gamma_s}}\left[\gamma_{gs}\right]_s - \left[\gamma_{ss}\right]_s\right)$; volatilization-dissolution between aqueous and gaseous phases in soil [SD39]

$Q_{dr\gamma_s} = \alpha_{gr_s} D_{d\gamma}\left(S'_\gamma f_{T_{d\gamma_s}}\left[\gamma_{gr}\right]_s - \left[\gamma_{sr}\right]_s\right)$; volatilization-dissolution between aqueous and gaseous phases in roots [SD40]

$Q_{gs\gamma,surf} = g_{a,surf}\left\{\left[\gamma_a\right] - \left\{2\left[\gamma_{gs}\right]_{surf} D_{gs\gamma,surf}/L_{surf} + g_{a,surf}\left[\gamma_a\right]\right\}/\left\{2D_{gs\gamma,surf}/L_{surf} + g_{a,surf}\right\}\right\}$; convective-conductive gas flux between soil surface and the atmosphere [SD41]

$Q_{gs\gamma_i} = -Q_{w_i}\left[\gamma_{gs}\right]_s + \frac{2D_{gs\gamma_i}\left(\left[\gamma_{gs}\right]_s - \left[\gamma_{gs}\right]_d\right)}{L_{s_i} + L_{d_i}}$; 3D convective-conductive gas flux between two adjacent grid cells [SD42]

$$Q_{gr\gamma_{i=z}} = \frac{D_{gr\gamma_{i=z}}\left(\left[\gamma_{gr}\right]_d - \left[\gamma_a\right]\right)}{\sum_{1,i=z} L_{d_{i=z}}}$$; convective-conductive gas flux between root and the atmosphere [SD43]

$$D_{gs\gamma_i} = \frac{D'_{g\gamma} f_{T_{g_s}} \left[0.5\left(\theta_{g_s} + \theta_{g_d}\right)\right]^2}{\theta_{P_s}^{0.67}}$$; 3D gaseous diffusivity between two adjacent grid cells as functions of air-filled porosities in those cells [SD44]

$$D_{gr\gamma_{i=z}} = \frac{D'_{g\gamma} f_{T_{g_s}} \theta_{pr_s}{}^{1.33} A_{r_s}}{A_{i=x,y}}$$; gaseous diffusivity as a function of air-filled porosity in the roots/mycorrhizae [SD45]

Where, subscripts *i*=dimensions (*i=x, y, z*), *s*=source cell, *d*=destination cell, *surf*=soil surface layer; $Q_{ds\gamma}$=volatilization – dissolution of gas γ between aqueous and gaseous phases in soil (g m^{-2} h^{-1}); α_{gs}=air-water interfacial area in soil (m^2 m^{-2}); $D_{d\gamma}$= volatilization - dissolution transfer coefficient for gas γ (m^2 h^{-1}); S'_γ =Ostwald solubility coefficient of gas γ at 30°C (0.0293 for $\gamma = O_2$) (Wilhelm et al., 1977); $f_{T_{d\gamma}}$ =temperature dependence of S'_γ (Wilhelm et al., 1977); [γ_{gs}]=gaseous concentration of gas γ in soil (g m^{-3}); [γ_{ss}]= aqueous concentration of gas γ in soil (g m^{-3}); $Q_{dr\gamma}$= volatilization – dissolution of gas γ between aqueous and gaseous phases in root/moss (g m^{-2} h^{-1}); α_{gr}= air-water interfacial area in root/mycorrhizae (m^2 m^{-2}) (Skopp, 1985); [γ_{gr}]= gaseous concentration of gas γ in root/mycorrhizae (g m^{-3}); [γ_{sr}]= aqueous concentration of gas γ in root/moss/mycorrhizae (g m^{-3}); $Q_{gs\gamma}$= gaseous flux of gas γ in soil (g m^{-2} h^{-1}); Q_w=sub-surface water flux (m^3 m^{-2} h^{-1}); $D_{gs\gamma}$=gaseous diffusivity of gas γ in soil (m^2 h^{-1}) (Millington and Quirk, 1960); *L*=thickness of grid cells (m); $Q_{gr\gamma}$=gaseous flux of gas γ between root/mycorrhizae and the atmosphere (m^2 h^{-1}); $D_{gr\gamma}$=gaseous diffusivity of gas γ in root/mycorrhizae (m^2 h^{-1}) (Luxmoore et al., 1970a,b); g_a = boundary layer conductance (m h^{-1}); [γ_a]=atmospheric concentration of gas γ (g m^{-3}); $D'_{g\gamma}$ =diffusivity of gas γ in air at 0°C (m^2 h^{-1}) (6.43×10^{-2} m^2 h^{-1} for γ=O_2) (Campbell, 1985); f_{T_g} =temperature dependence of $D'_{g\gamma}$ (Campbell, 1985); θ_g=air-filled porosity (m^3 m^{-3}); θ_P=total porosity of soil (m^3 m^{-3}); θ_{pr}= root/mycorrhizal porosity representing aerenchyma fraction (m^3 m^{-3}); A_r= root cross-sectional area (m^2); and *A*=area of landscape position (m^2).

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Table S1. Statistics from regressions between hourly modelled and gap-filled CO_2 fluxes from 2004-2009 at a Western Canadian fen peatland

(a) Regressions of modelled vs. gap-filled net ecosystem CO_2 fluxes over whole years of 2004-2008[a]

Year	Total annual precipitation (mm)	*n*	*a*	*b*	R^2	RMSE (μmol m^{-2} s^{-1})
2004	553	3750	-0.13	1.20	0.89	0.64
2005	387	2807	-0.49	1.03	0.76	0.82
2006	465	2748	-0.48	1.15	0.81	0.58
2007	431	3375	-0.36	0.97	0.74	1.23
2008	494	2941	-0.54	1.05	0.79	0.95

(b) Regressions of modelled vs. gap-filled net ecosystem CO_2 fluxes over growing seasons (May-August) of 2004-2009

Year	Total growing season precipitation (mm)	*n*	*a*	*b*	R^2	RMSE (μmol m^{-2} s^{-1})
2004	287	837	-0.01	1.21	0.87	1.22
2005	276	680	-0.57	1.07	0.75	1.26
2006	253	773	-1.70	0.95	0.73	0.78
2007	237	1058	-0.51	0.98	0.76	1.88
2008	276	810	-1.04	1.02	0.79	1.62
2009	138	1010	-0.02	0.98	0.87	1.20

(*a, b*) from simple linear regressions of modelled on gap-filled, and R^2 = coefficient of determination; RMSE = root mean square for errors from simple linear regressions of gap-filled on simulated; [a] whole year modelled vs. gap-filled CO_2 flux regression for 2009 could not be done due to the lack of gap-filling (arose from long gap in measurements) from September to December in that year.