Supplement of

Coupled eco-hydrology and biogeochemistry algorithms enable the simulation of water table depth effects on boreal peatland net CO₂ exchange

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Supplementary material

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

Decomposition

\[ D_{Si,j,C} = D'_{Si,j,C} M_{i,d,t,C} f_{fg}(S_{i,t,C} / G_{i,t,C}) \]
\[ D_{Zi,j,L} = D'_{Zi,j,C} M_{i,d,t,C} f_{fg}(Z_{i,t,C} / G_{i,t,C}) \]
\[ D_{A_i,j,L} = D'_{A_i,j,C} M_{i,d,t,C} f_{fg}(A_{i,t,C} / G_{i,t,C}) \]
\[ S_{i,t,C} = \sum_j S_{i,j,t,C} \]
\[ Z_{i,t,C} = \sum_j Z_{i,j,t,C} \]
\[ G_{i,t,C} = S_{i,t,C} + Z_{i,t,C} + A_{i,t,C} \]
\[ M_{i,d,t,C} = M_{i,a,t,C} + q_w (M_{i,a,t,C} G_{i,t,C} - M_{i,a,t,C} G_{i,t,C})(G_{i,t,C} + G_{i,t,C}) \]
\[ M_{i,a,t,C} = \sum_m M_{i,m,a,t,C} \]
\[ D'_{Si,j,t,C} = \{D_{Si,j,C}[S_{i,j,t,C}]/[S_{i,j,t,C}] + K_{ma}(1.0 + [\sum M_{i,d,t,C}]/K_{ma}) \} \]
\[ D'_{Zi,j,t,C} = \{D_{Zi,j,C}[Z_{i,j,t,C}]/[Z_{i,j,t,C}] + K_{ma}(1.0 + [M_{i,d,t,C}]/K_{ma}) \} \]
\[ D'_{A_i,j,t,C} = \{D_{A_i,j,C}[A_{i,t,C}]/[A_{i,t,C}] + K_{ma}(1.0 + [M_{i,d,t,C}]/K_{ma}) \} \]
\[ \delta S_{i,j,t,C}/\delta t = \beta \sum_n (U_{i,n,C} - R_{nil}) \left( S'_{i,j,k,C} / S'_{i,j,t,C} \right) \{S'_{i,j,k,C}/S_{i,j,t,C} + K_{a} \} \]
\[ f_{fg} = T_a \{e^{R_a (RT_a)}\} / \{1 + e^{H_a - ST_{a}} / (RT_{a})\} + e^{(S_{i,j,k,C} - H_{a}) / (RT_{a})} \]

decomposition of litter, POC, humus

decomposition of microbial residues

decomposition of adsorbed SOC

total C in all kinetic components of litter, POC, humus

total C in all kinetic components of microbial residues

total C in substrate-microbe complexes

Redistribution of active microbial biomass from each substrate-microbe complex \(i\) to other substrate-microbe complexes \(ix\) according to concentration differences (priming)

Substrate and water constraint on \(D\) from colonized litter, POC and humus, microbial residues and adsorbed SOC

Colonized litter determined by microbial growth into uncolonized litter

Arrhenius function for \(D\) and \(R_h\)
$D_{Ni,j,n,p} = D_{Ni,j,C}(S_{Ni,j,n,p}/S_{Ni,j,C})$

$D_{Zi,j,n,p} = D_{Zi,j,C}(Z_{i,j,n,p}/Z_{i,j,C})$

$D_{Ni,j,n,p} = D_{Ni,j,C}(A_{i,n,j,p}/A_{i,j,C})$

$Y_{i,j,C} = k_u(G_{i,j,C} F_i(\Delta Q_{i,j,C})^b - X_{i,j,C})$

$Y_{i,j,n,p} = Y_{i,j,C}(Q_{i,j,n,p}/Q_{i,j,C})$

$Y_{i,j,n,p} = Y_{i,j,C}(X_{i,j,n,p}/X_{i,j,C})$

**Microbial growth**

$R_{n} = \Sigma_{i,j} \Sigma_{f} R_{j,i,n,l}$

$R_{j,i,n,l} = R'_{j,i,n,l} \min\{C_{Ni,n,l,0}/C_{Ni}, C_{P_{i,n,l,0}/C_{P_{i}}}\}$

$R_{j,i,n,l} = M_{i,n,j,C} \cdot \{R_{j,i,n,l}[Q_{i,j,C}]/\{(K_{moc} + [Q_{i,j,C}])\}f_{j,i,l}/f_{j,i,l}^g\}$

$R_{j,i,n,l} = R'_{j,i,n,l}(U_{02,j,n,l}/U_{02,j,n,l})$

$f_{j,i,l} = 1.0 - 6.67(1.0 - e^{M_{i,j} d_{j,i} R_{j,i,n,l}})$

$U_{02,j,n,l} = 2.67 R_{j,i,n,l}$

$U_{02,j,n,l} = U_{02,j,n,l}[O_{2m,n,l}]/([O_{2m,n,l}] + K_{O_{2}})$

$\psi_{j} constraints on microbial growth$

$U_{02,j,n,l} = U_{02,j,n,l}[O_{2m,n,l}]/([O_{2m,n,l}] + K_{O_{2}})$

$R_{m,i,j,n,l} = R_{m}M_{i,n,j,l}\Sigma_{f} f_{m,n}$

$f_{m,n} = e^{[\psi_{j} d_{j,i} - 298.16]}$

$R_{g,i,j} = R_{j,i,n,l} - \Sigma_{j} R_{m,i,j,n,l}$

$U_{j,n,C} = \min(R_{j,i,n,l}, \Sigma_{j} R_{m,i,j,n,l}) + R_{g,i,j} (1 + \Delta G_{j}/E_{m})$

$U_{j,n,n,p} = U_{j,n,C} Q_{j,n,n,p}/Q_{j,n,C}$

$D_{Mj,n,j,C} = D_{Mj,C} M_{j,n,j,C} f_{g}$

N and P coupled with C during $D$ [SA7a]

Freundlich sorption of DOC [SA8]

$Y_{i,j,C} > 0 \quad$ adsorption of DON, DOP [SA9]

$Y_{i,j,C} < 0 \quad$ desorption of DON, DOP [SA10]

$R_{n} constrained by microbial N, P$ [SA11]

$R_{n} constrained by substrate DOC$ [SA12]

$R_{n} constrained by O_{2}$ [SA13]

O$_{2}$ demand driven by potential $R_{n}$ [SA14]

active uptake coupled with radial diffusion of O$_{2}$ [SA15]

$\Delta$C uptake driven by $R_{g}$ [SA16]

DON,DOP uptake driven by $U_{j,n,C}$ [SA17a]

first-order decay of microbial C, [SA17b]
Microbial nutrient exchange

\[ D_{M,i,n,l,P} = D_{M,0} \frac{M_{i,n,l,P}}{f_{i,n,l,P}} \]

\[ \delta M_{i,n,l,C}/\delta t = F_j U_{i,n,l} - F_j R_{i,n,l} - D_{M,i,n,l,C} \]

\[ \delta M_{i,n,l,C}/\delta t = F_j U_{i,n,l} - R_{i,n,l} - D_{M,i,n,l,C} \]

**Microbial nutrient exchange**

\[ U_{\text{NH}_4,n,l,i} = (M_{i,n,l,C} C_{i,j} - M_{i,n,l,C}) \]

\[ U_{\text{NH}_4,n,l,i} = \text{min} \{ (M_{i,n,l,C} C_{i,j} - M_{i,n,l,C}), \]

\[ U_{\text{NO}_3,n,l,i} = (M_{i,n,l,C} C_{i,j} - (M_{i,n,l,C} + U_{\text{NH}_4,i,n,l,j}))) \]

\[ U_{\text{PO}_4,n,l,i} = (M_{i,n,l,C} C_{i,j} - M_{i,n,l,C}) \]

\[ U_{\text{PO}_4,n,l,i} = \text{min} \{ (M_{i,n,l,C} C_{i,j} - M_{i,n,l,C}), \]

\[ \Phi_{n,f,j,l} = \text{max} \{ 0, M_{i,n-f,j,l,C} C_{i,n-l} - M_{i,n-f,j,l,N} - \text{max} \{ 0, U_{i,n-f,j,l,N} \} \}

\[ R \Phi_{n,f,j,l} = E \Phi_{n,f,j,l} \]

\[ \delta M_{i,n,l,N}/\delta t = F_j U_{i,n,l,N} + U_{\text{NH}_4,i,n,l,i} + U_{\text{NO}_3,i,n,l,i} + \Phi_{n,f,j,l} - D_{M,i,n,l,N} \]

\[ \delta M_{i,n,l,P}/\delta t = F_j U_{i,n,l,P} + U_{\text{PO}_4,i,n,l,i} - D_{M,i,n,l,P} \]

\[ M_{i,n,a,l,C} = M_{i,n,a,l-C} \text{labile, } i,C + M_{i,n,a,l-resistant, l,C} F_0/F_i \]

\[ \text{partial release of microbial N, P} \]

\[ [R_{\text{i,0,l}} > R_{\text{mu,n,i,l}}] \] growth \[ [R_{\text{i,0,l}} < R_{\text{mu,n,i,l}}] \] senescence

\[ U_{\text{NH}_4} < 0 \] mineralization \[ U_{\text{NH}_4} > 0 \] immobilization

\[ U_{\text{NO}_3} > 0 \] immobilization \[ U_{\text{PO}_4} < 0 \] mineralization

\[ U_{\text{PO}_4} > 0 \] immobilization

N\text{fixation driven by N deficit of diazotrophic population}

growth vs. losses of microbial N, P

Humification

\[ H_{S,i,j} = 1 \text{gmoi, l,C} = D_{S,i,j} \text{gmoi, l,C} \]

\[ H_{S,i,j} = 1 \text{gmoi, l,N.P} = D_{S,i,j} \text{gmoi, l,N,P} \]

\[ H_{S,i,j} = 1 \text{gmoi, l,C} = H_{S,i,j} \text{gmoi, l,C} L_{i,j} \]

\[ H_{S,i,j} = 1 \text{gmoi, l,N,P} = H_{S,i,j} \text{gmoi, l,C} S_{i,j,l,N,P}/S_{i,j,l,C} \]

decomposition products of litter added to POC depending on lignin

[SA24]

[SA25a]

[SA25b]

[SA26a]

[SA26b]

[SA26c]

[SA26d]

[SA26e]

[SA27]

[SA28]

[SA29a]

[SA29b]

[SA30]

[SA31]

[SA32]

[SA33]

[SA34]
\[ H_{M_{i,n,j,l,C}} = D_{M_{i,n,j,l,C}} F_h \]
\[ H_{M_{i,n,j,N,P}} = H_{M_{i,n,j,l,C}} \frac{M_{i,n,j,l,N,P}}{M_{i,n,j,l,C}} \]

decomposition products of microbes added to humus depending on clay [SA35]

definition of variables in Appendix A

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( i )</td>
<td>substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus.</td>
<td>( i )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( j )</td>
<td>kinetic component: labile ( l ), resistant ( r ), active ( a )</td>
<td>( j )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( l )</td>
<td>soil or litter layer</td>
<td>( l )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( n )</td>
<td>microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)</td>
<td>( n )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Subscripts**

**Variables**

\( A_{i,l,C} \) mass of adsorbed SOC \( g \ C \ m^{-2} \)

\([A_{i,l,C}]\) concentration of adsorbed SOC in soil \( g \ C \ M_{-1} \)

\( a \) microbial surface area \( m^{2} \)

\( B \) parameter such that \( f_{eq} = 1.0 \) at \( T_l = 298.15 \) K \( 26.230 \)

\( b \) Freundlich exponent for sorption isotherm \( 0.85 \) (Grant et al., 1993a, b)

\( \beta \) specific colonization rate of uncolonized substrate \( 2.5 \) (Grant et al., 2010)

\( C_{N,P,i,n,a,l} \) ratio of \( M_{i,n,a,N,P} \) to \( M_{i,n,a,C} \) \( g \ N \) or \( P \) g C\(^{-1} \)

\( C_{N,P,j} \) 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)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_{Mi,j}$</td>
<td>specific decomposition rate of $M_{i,n,j}$ at 30°C</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>0.0125 and 0.00035 for $j =$ labile and resistant, respectively</td>
<td>(Grant et al., 1993a, b)</td>
</tr>
<tr>
<td>$D_{Mi,n,j,IC}$</td>
<td>decomposition rate of $M_{i,n,j,IC}$</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Mi,n,j,NP}$</td>
<td>decomposition rate of $M_{i,n,j,NP}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{O2l}$</td>
<td>aqueous dispersivity–diffusivity of O$_2$ during microbial uptake in soil</td>
<td>m$^2$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Ai,j,C}$</td>
<td>decomposition rate of $A_{i,j,C}$ by $M_{i,d,l,C}$ producing $Q$ [SA13]</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Ai,j,NP}$</td>
<td>decomposition rate of $A_{i,j,NP}$ by $M_{i,d,l,C}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Si,j,IC}$</td>
<td>specific decomposition rate of $S_{i,j,IC}$ by $\Sigma M_{i,n,a,l}$ at 25°C and producing $Q$ [SA13]</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>1.0, 1.0, 0.15, and 0.025 for $j =$ protein, carbohydrate, cellulose, and lignin</td>
<td>(Grant et al., 1993a, b)</td>
</tr>
<tr>
<td>$D_{Si,j,NP}$</td>
<td>decomposition rate of $S_{i,j,NP}$ by $\Sigma M_{i,n,a,l}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Zi,j,IC}$</td>
<td>specific decomposition rate of $Z_{i,j,IC}$ by $\Sigma M_{i,n,a,l}$ at 25°C and producing $Q$ in [SA13]</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>0.25 and 0.05 for $j =$ labile and resistant biomass</td>
<td>(Grant et al., 1993a, b)</td>
</tr>
<tr>
<td>$D_{Zi,j,NP}$</td>
<td>decomposition rate of $Z_{i,j,NP}$ by $\Sigma M_{i,n,a,l}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
$\Delta G_x$  
energy yield of C oxidation with different reductants $x$  
kJ g C$^{-1}$  
37.5 ($x = O_2$); 4.43 ($x = $DOC)

$E_m$  
energy requirement for growth of $M_{i,n,l}$  
kJ g C$^{-1}$  
25

$E_{\phi}$  
energy requirement for non-symbiotic N$_2$ fixation by heterotrophic diazotrophs ($n = f$)  
g C g N$^{-1}$  
5  
(Waring and Running, 1998)

$F_h$  
fraction of products from microbial decomposition that are humified (function of clay content)  
$0.167 + 0.167 \times $clay

$F_i$  
fraction of microbial growth allocated to labile component $M_{i,n,l}$  
0.55  
(Grant et al., 1993a, b)

$F_r$  
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 $H_{i,l,C}$

$f_{d,n,l,N,P}$  
fraction of N or P released with $D_{M_{i,n,l,l,C}}$ during decomposition  
dimensionless  
0.33  
$U_{NH4} > 0$

1.00  
$U_{NH4} < 0$

0.33  
$U_{PO4} > 0$

1.00  
$U_{PO4} < 0$

$f_{ggl}$  
temperature function for microbial growth respiration  
dimensionless

$f_{ml}$  
temperature function for maintenance respiration  
dimensionless

$f_{wgl}$  
soil water potential function for microbial, root or mycorrhizal growth respiration  
dimensionless  
(Pirt, 1975)

$q_{n=f,j,l}$  
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$_2$PO$_4^-$ in soil solution  
g P m$^{-3}$
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_a$</td>
<td>energy of activation</td>
<td>J mol$^{-1}$</td>
<td>65 x 10$^3$</td>
<td>(Addiscott, 1983)</td>
</tr>
<tr>
<td>$H_{dh}$</td>
<td>energy of high temperature deactivation</td>
<td>J mol$^{-1}$</td>
<td>225 x 10$^3$</td>
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</tr>
<tr>
<td>$H_{dl}$</td>
<td>energy of low temperature deactivation</td>
<td>J mol$^{-1}$</td>
<td>198 x 10$^3$</td>
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</tr>
<tr>
<td>$H_{M_i,n,j,C}$</td>
<td>transfer of microbial C decomposition products to humus</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_{M_i,n,j,N,P}$</td>
<td>transfer of microbial N or P decomposition products to humus</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_{S_i,j,C}$</td>
<td>transfer of C hydrolysis products to particulate OM</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_{S_i,j,N,P}$</td>
<td>transfer of N or P hydrolysis products to particulate OM</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K_{iS}$</td>
<td>inhibition constant for microbial colonization of substrate</td>
<td>-</td>
<td>0.5</td>
<td>(Grant et al., 2010)</td>
</tr>
<tr>
<td>$K_{NH_4}$</td>
<td>M-M constant for NH$_4^+$ uptake at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td>0.40</td>
<td></td>
</tr>
<tr>
<td>$K_{NO_3}$</td>
<td>M-M constant for NO$_3^-$ uptake at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td>0.35</td>
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<tr>
<td>$K_{PO_4}$</td>
<td>M-M constant for H$_2$PO$_4^-$ uptake at microbial surfaces</td>
<td>g P m$^{-3}$</td>
<td>0.125</td>
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<tr>
<td>$K_{iD}$</td>
<td>inhibition constant for $[M_{i,n,a}]$ on $S_{i,C}, Z_{i,C}$</td>
<td>g C m$^{-3}$</td>
<td>25</td>
<td>(Lizama and Suzuki, 1991; Grant et al., 1993a, b)</td>
</tr>
<tr>
<td>$K_{NaD}$</td>
<td>Michaelis–Menten constant for $D_{S_i,j,C}$</td>
<td>g C Mg$^{-1}$</td>
<td>75</td>
<td></td>
</tr>
<tr>
<td>$K_{NaQ_C}$</td>
<td>Michaelis–Menten constant for $R'<em>{h</em>{i,a}}$ on $[Q_{i,C}]$</td>
<td>g C m$^{-3}$</td>
<td>36</td>
<td></td>
</tr>
<tr>
<td>$K_{O_2}$</td>
<td>Michaelis–Menten constant for reduction of O$_2$s by microbes, roots and mycorrhizae</td>
<td>g O$_2$ m$^{-3}$</td>
<td>0.064</td>
<td>(Griffin, 1972)</td>
</tr>
<tr>
<td>$k_{is}$</td>
<td>equilibrium rate constant for sorption</td>
<td>h$^{-1}$</td>
<td>0.01</td>
<td>(Grant et al., 1993a, b)</td>
</tr>
<tr>
<td>$L_{hi}$</td>
<td>ratio of nonlignin to lignin components in humified hydrolysis products</td>
<td></td>
<td>0.10, 0.05, and 0.05 for $j$ = protein, carbohydrate, and cellulose, respectively</td>
<td>(Schulten and Schnitzer, 1997)</td>
</tr>
<tr>
<td>$M$</td>
<td>molecular mass of water</td>
<td>g mol$^{-1}$</td>
<td>18</td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
<td></td>
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<tr>
<td>------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{i,d,l,C}$</td>
<td>heterotrophic microbial C used for decomposition</td>
<td>g C m$^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{i,n,j,i,C}$</td>
<td>microbial C</td>
<td>g C m$^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{i,n,j,i,N}$</td>
<td>microbial N</td>
<td>g N m$^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{i,n,j,i,P}$</td>
<td>microbial P</td>
<td>g P m$^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M_{i,n,a,i,C}$</td>
<td>active microbial C from heterotrophic population $n$ associated with $G_{i,l,C}$</td>
<td>g C m$^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[M_{i,n,a,i,C}]$</td>
<td>concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,i,C}/\theta$</td>
<td>g C m$^{-3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[\text{NH}<em>4^+</em>{i,n,j,l}]$</td>
<td>concentration of $\text{NH}_4^+$ at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[\text{NH}<em>4^+</em>{\text{mn}}]$</td>
<td>concentration of $\text{NH}<em>4^+$ at microbial surfaces below which $U</em>{\text{NH}_4} = 0$</td>
<td>g N m$^{-3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[\text{NO}<em>3^-</em>{i,n,j,l}]$</td>
<td>concentration of $\text{NO}_3^-$ at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[\text{NO}<em>3^-</em>{\text{mn}}]$</td>
<td>concentration of $\text{NO}<em>3^-$ at microbial surfaces below which $U</em>{\text{NO}_3} = 0$</td>
<td>g N m$^{-3}$</td>
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<tr>
<td>$[\text{H}_2\text{PO}<em>4^-</em>{i,n,j,l}]$</td>
<td>concentration of $\text{H}_2\text{PO}_4^-$ at microbial surfaces</td>
<td>g N m$^{-3}$</td>
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<tr>
<td>$[\text{H}_2\text{PO}<em>4^-</em>{\text{mn}}]$</td>
<td>concentration of $\text{H}_2\text{PO}<em>4^-$ at microbial surfaces below which $U</em>{\text{PO}_4} = 0$</td>
<td>g N m$^{-3}$</td>
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<td></td>
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<tr>
<td>$[O_{2\text{m,n,i}}]$</td>
<td>O$_2$ concentration at heterotrophic microsites</td>
<td>g O$_2$ m$^{-3}$</td>
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<td></td>
</tr>
<tr>
<td>$[O_{2d}]$</td>
<td>O$_2$ concentration in soil solution</td>
<td>g O$_2$ m$^{-3}$</td>
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<tr>
<td>$Q_{i,l,C}$</td>
<td>DOC from products of $D_{i,j,i,C}$ [SA3] and $D_{i,j,i,C}$ [SA5]</td>
<td>g C m$^{-2}$</td>
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<td>$[Q_{i,l,C}]$</td>
<td>solution concentration of $Q_{i,l,C}$</td>
<td>g C Mg$^{-1}$</td>
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<td></td>
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<tr>
<td>$Q_{i,N,P}$</td>
<td>DON and DOP from products of $(D_{i,j,i,N,P} + D_{i,j,i,N,P})$</td>
<td>g N or P m$^{-2}$</td>
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<td>$q_m$</td>
<td>constant for reallocating $M_{i,a,l,C}$ to $M_{i,d,l,C}$</td>
<td>- 0.5</td>
<td></td>
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</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
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<td>-----------------------------------------------------------------------------</td>
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<tr>
<td>( R )</td>
<td>gas constant</td>
<td>( \text{J mol}^{-1} \text{K}^{-1} )</td>
<td>8.3143</td>
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<tr>
<td>( R_{i,n,f,j,l} )</td>
<td>respiration for non-symbiotic ( \text{N}_2 ) fixation by heterotrophic diazotrophs ((n = f))</td>
<td>( \text{g C m}^{-2} \text{h}^{-1} )</td>
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<tr>
<td>( R_{gi,n,l} )</td>
<td>growth respiration of ( M_{i,n,a,l} ) on ( Q_{i,l,C} ) under nonlimiting ( \text{O}_2 ) and nutrients</td>
<td>( \text{g C g}^{-1} \text{h}^{-1} )</td>
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<tr>
<td>( R_{h} )</td>
<td>total heterotrophic respiration of all ( M_{i,n,a,l} ) under ambient DOC, ( \text{O}_2 ), nutrients, ( \theta ) and temperature</td>
<td>( \text{g C m}^{-2} \text{h}^{-1} )</td>
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<tr>
<td>( R_{ui,n,l} )</td>
<td>heterotrophic respiration of ( M_{i,n,a,l} ) under ambient DOC, ( \text{O}_2 ), nutrients, ( \theta ) and temperature</td>
<td>( \text{g C m}^{-2} \text{h}^{-1} )</td>
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<tr>
<td>( R_{bi,n,l} )</td>
<td>specific heterotrophic respiration of ( M_{i,n,a,l} ) under nonlimiting ( \text{O}_2 ), DOC, ( \theta ) and 25°C</td>
<td>( \text{g C g}^{-1} \text{h}^{-1} )</td>
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<tr>
<td>( R_{bi,n,l}^{'} )</td>
<td>specific heterotrophic respiration of ( M_{i,n,a,l} ) under nonlimiting DOC, ( \text{O}_2 ), nutrients, ( \theta ) and 25°C</td>
<td>( \text{g C g}^{-1} \text{h}^{-1} )</td>
<td>0.125</td>
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<tr>
<td>( R_{ui,n,l}^{'} )</td>
<td>heterotrophic respiration of ( M_{i,n,a,l} ) under nonlimiting ( \text{O}_2 ) and ambient DOC, nutrients, ( \theta ) and temperature</td>
<td>( \text{g C m}^{-2} \text{h}^{-1} )</td>
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<tr>
<td>( R_{m} )</td>
<td>specific maintenance respiration at 25°C</td>
<td>( \text{g C g}^{-1} \text{h}^{-1} )</td>
<td>0.0115</td>
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<tr>
<td>( R_{ni,n,j,l} )</td>
<td>maintenance respiration by ( M_{i,n,j,l} )</td>
<td>( \text{g C m}^{-2} \text{h}^{-1} )</td>
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<td></td>
</tr>
<tr>
<td>( r_{wl} )</td>
<td>radius of ( r_m + ) water film at current water content</td>
<td>( \text{m} )</td>
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<td></td>
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<tr>
<td>( r_m )</td>
<td>radius of heterotrophic microsite</td>
<td>( \text{m} )</td>
<td>2.5 \times 10^{-6}</td>
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<tr>
<td>( r_{wl} )</td>
<td>thickness of water films</td>
<td>( \text{m} )</td>
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</tr>
<tr>
<td>( S )</td>
<td>change in entropy</td>
<td>( \text{J mol}^{-1} \text{K}^{-1} )</td>
<td>710</td>
<td></td>
</tr>
<tr>
<td>( [S_{i,j,l,C}] )</td>
<td>concentration of ( S_{i,j,l,C} ) in soil</td>
<td>( \text{g C Mg}^{-1} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( S_{i,j,l,C} )</td>
<td>mass of colonized litter, POC or humus C</td>
<td>( \text{g C m}^{-2} )</td>
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<td></td>
</tr>
<tr>
<td>( S'_{i,j,l,C} )</td>
<td>mass of uncolonized litter, POC or humus C</td>
<td>( \text{g C m}^{-2} )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(Shields et al., 1973)
$S_{i,j,N,P}$ mass of litter, POC or humus N or P  g N or P m$^{-2}$

$T_d$ soil temperature K

$U_{i,n,C}$ uptake of $Q_{i,C}$ by $\Sigma_m M_{i,n,a,l}$ under limiting nutrient availability g C m$^{-2}$ h$^{-1}$

$U_{i,n,N,P}$ uptake of $Q_{i,N,P}$ by $\Sigma_m M_{i,n,a,l}$ under limiting nutrient availability g N or P m$^{-2}$ h$^{-1}$

$U_{NH4,n,i,l}$ NH$_4^+$ uptake by microbes g N m$^{-2}$ h$^{-1}$

$U'_{NH4}$ maximum $U_{NH4}$ at 25 °C and non-limiting NH$_4^+$ g N m$^{-2}$ h$^{-1}$ 5.0 x 10$^{-3}$

$U_{NO3,n,i,l}$ NO$_3^-$ uptake by microbes g N m$^{-2}$ h$^{-1}$

$U'_{NO3}$ maximum $U_{NO3}$ at 25 °C and non-limiting NO$_3^-$ g N m$^{-2}$ h$^{-1}$ 5.0 x 10$^{-3}$

$U_{O2,i,n}$ O$_2$ uptake by $M_{i,n,a,l}$ under ambient O$_2$ g m$^{-2}$ h$^{-1}$

$U'_{O2,i,n}$ O$_2$ uptake by $M_{i,n,a,l}$ under nonlimiting O$_2$ g m$^{-2}$ h$^{-1}$

$U_{PO4,n,i,l}$ H$_2$PO$_4^-$ uptake by microbes g N m$^{-2}$ h$^{-1}$

$U'_{PO4}$ maximum $U_{PO4}$ at 25 °C and non-limiting H$_2$PO$_4^-$ g N m$^{-2}$ h$^{-1}$ 5.0 x 10$^{-3}$

$X_{i,C}$ adsorbed C hydrolysis products g C Mg$^{-1}$

$X_{i,N,P}$ adsorbed N or P hydrolysis products g P Mg$^{-1}$

$y$ selected to give a $Q_{10}$ for $f_{tm}$ of 2.25 0.081

$\psi_s$ soil or residue water potential MPa

$Y_{i,C}$ sorption of C hydrolysis products g C m$^{-2}$ h$^{-1}$

$Y_{i,N,P}$ sorption of N or P hydrolysis products g P m$^{-2}$ h$^{-1}$

$[Z_{i,j,i,C}]$ concentration of $Z_{i,j,i,C}$ in soil g C Mg$^{-1}$
\( Z_{i,j,C} \) mass of microbial residue C in soil  \( \text{g C m}^{-2} \)

\( Z_{i,j,N,P} \) mass of microbial residue N or P in soil  \( \text{g P m}^{-2} \)
Appendix B: Soil-plant water relations

Canopy transpiration

\[ R_{\text{ct}} + L_{\text{ct}} + H_{\text{ct}} + G_{\text{ct}} = 0 \]

\[ L_{\text{ct}} = L \left( e_a - e_{\text{ct}(T_a,T_e)} \right) / r_{\text{ct}} \]

\[ L_{\text{ct}} = L \left( e_a - e_{\text{ct}(T_a,T_e)} \right) / (r_{\text{ct}} + r_{\text{ci}}) - L_{\text{et}} \]  

[SB1b]

\[ H_{\text{ct}} = \rho C_{\theta}(T_a - T_e) / r_{\text{ct}} \]

\[ r_{\text{cmin}} = 0.64 \left( C_b - C'_{\text{bi}} \right) / V_{\text{ci}} \]

\[ r_{\text{ci}} = r_{\text{cmin}} + (r_{\text{cmax}} - r_{\text{cmin}}) e^{(-r_{\text{ci}})} \]

\[ r_{\text{ci}} = \{(\ln(z_n - z_0) / z_0) / K^2 \mu_0 \} / (1 - 10 R_i) \]

\[ R_i = \{g (z_n - z_0)(u_x^2 T_a) / (T_a - T_e) \} \]

\[ \psi_{\text{ci}} = \psi_{\text{ci}} - \psi_{\text{ci}} \]

Root/moss/mycorrhizal water uptake

\[ U_{\text{ui}} = \Sigma \Sigma U_{\text{ui,ri}} \]

\[ U_{\text{ui,ri}} = (\psi_{\text{ri}} - \psi_{\text{ri}}) / (\Omega_{\text{ui,ri}} + \Omega_{\text{oi,ri}} + \Sigma \Omega_{\text{ui,ri,ri}}) \]

\[ \psi_{\text{ri}} = \psi_{\text{ri}} + 0.01 \, z_{\text{ui}} \]

\[ \psi_{\text{ri}} = \psi_{\text{ri}} - 0.01 \, z_{\text{ri}} \]

\[ \Omega_{\text{ui,ri}} = \ln \{(d_{\text{ri,ri}} / r_{\text{ri,ri}}) / (2 \pi L_{\text{ri,ri}} K_{\text{ri,ri}}) \} / \theta_{\text{ri}} \]

\[ \Omega_{\text{ui,ri}} = \mathbf{\Psi} \, r_{\text{ri}} / L_{\text{ri}} \]

\[ \Omega_{\text{ui,ri,ri-1}} = \mathbf{\Psi} \, r_{\text{ri}} / n_{\text{ri,ri-1}} (r_{\text{ri,ri-1}} / r_{\text{ri,ri}})^3 \]

\[ \mathbf{\Psi} \, r_{\text{ri}} / n_{\text{ri,ri-1}} (r_{\text{ri,ri-1}} / n_{\text{ri,ri}})^3 \Sigma_{\text{ri,ri}} (M_{\text{ri,ri}}) / M_{\text{ri,ri}} \]

\[ \Omega_{\text{ui,ri,ri-2}} = \mathbf{\Psi} \, r_{\text{ri}} / n_{\text{ri,ri-2}} (r_{\text{ri,ri-2}} / r_{\text{ri,ri}})^3 \]

\[ \partial L_{\text{ri,ri}} / \partial t = \delta M_{\text{ri,ri}} / \partial t \, \nu_{\text{ri}} / \{\partial r / \partial \theta_{\text{ri}} (1 - \theta_{\text{pi,ri}}) (\pi r_{\text{ri,ri}})^2 \} \]

Canopy water potential

\[ (e_a - e_{\text{ct}(T_a)}) / (r_{\text{ct}} + r_{\text{ci}}) \]  

[SB1]  

\[ \psi_{\text{c}} \]  

[SB14]  

\[ \psi_{\text{c}} \]  

[SB1-14] equals uptake from [SB5-SB13] + change in storage
### Definition of variables in Appendix B

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Equation</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$I$</td>
<td>plant species or functional type: coniferous, deciduous, annual, perennial, $C_3$, $C_4$, monocot, dicot etc.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$J$</td>
<td>branch or tiller</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$K$</td>
<td>Node</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$L$</td>
<td>soil or canopy layer</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$M$</td>
<td>leaf azimuth</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>leaf inclination</td>
<td></td>
<td></td>
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<td></td>
</tr>
<tr>
<td>$o$</td>
<td>leaf exposure (sunlit vs. shaded)</td>
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<td></td>
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</tr>
<tr>
<td>$r$</td>
<td>root/moss/mycorrhizae</td>
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<td></td>
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</tr>
</tbody>
</table>

#### Subscripts

$I$  
$J$  
$K$  
$L$  
$M$  
$n$  
$o$  
$r$

#### Variables

- $\beta$: stomatal resistance shape parameter  
  Unit: MPa\(^{-1}\)  
  Equation: $-5.0$  
  Reference: (Grant and Flanagan, 2007)

- $C_b$: [CO\(_2\)] in canopy air  
  Unit: \(\mu\text{mol mol}^{-1}\)

- $C_i'$: [CO\(_2\)] in canopy leaves at $\psi_{c_i} = 0$ MPa  
  Unit: \(\mu\text{mol mol}^{-1}\)  
  Equation: $0.70 C_b$  
  Reference: (Larcher, 2003)

- $d_{i,r,l}$: half distance between adjacent roots/mosses  
  Unit: m

- $E_{ci}$: canopy transpiration  
  Unit: m\(^3\) m\(^{-2}\) h\(^{-1}\)

- $e_a$: atmospheric vapor density at $T_a$ and ambient humidity  
  Unit: g m\(^{-3}\)

- $e_{ci}(T_{ci},\psi_{ci})$: canopy vapor density at $T_{ci}$ and $\psi_{ci}$  
  Unit: g m\(^{-3}\)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>$G_{ci}$</td>
<td>canopy storage heat flux</td>
<td>W m(^{-2})</td>
</tr>
<tr>
<td>$H_{ki}$</td>
<td>canopy sensible heat flux</td>
<td>W m(^{-2})</td>
</tr>
<tr>
<td>$K$</td>
<td>von Karman’s constant</td>
<td>0.41</td>
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<tr>
<td>$\kappa_{ir,l}$</td>
<td>hydraulic conductivity between soil and root/moss surface</td>
<td>m(^2) MPa(^{-1}) h(^{-1})</td>
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<tr>
<td>$\gamma$</td>
<td>scaling factor for bole axial resistance from primary root/moss axial resistance</td>
<td>-</td>
</tr>
<tr>
<td>$L$</td>
<td>latent heat of evaporation</td>
<td>J g(^{-1})</td>
</tr>
<tr>
<td>$LE_{ci}$</td>
<td>latent heat flux between canopy and atmosphere</td>
<td>W m(^{-2})</td>
</tr>
<tr>
<td>$L_{i,r,l}$</td>
<td>length of roots/mosses/mycorrhizae</td>
<td>m m(^{-2})</td>
</tr>
<tr>
<td>$M_{i,r,l}$</td>
<td>mass of roots/mosses/mycorrhizae</td>
<td>g m(^{-2})</td>
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<tr>
<td>$n_{i,r,l,x}$</td>
<td>number of primary (x = 1) or secondary (x = 2) axes</td>
<td>m(^2)</td>
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<tr>
<td>$\Omega_{alr}$</td>
<td>axial resistivity to water transport along root/moss/mycorrhizal axes</td>
<td>MPa h m(^{-4})</td>
</tr>
<tr>
<td>$\Omega_{alr,l,x}$</td>
<td>axial resistance to water transport along axes of primary (x = 1) or secondary (x = 2) roots/mosses/mycorrhizae</td>
<td>MPa h m(^{-1})</td>
</tr>
<tr>
<td>$\Omega_{rilr}$</td>
<td>radial resistivity to water transport from surface to axis of roots/mosses/mycorrhizae</td>
<td>MPa h m(^{-2})</td>
</tr>
<tr>
<td>$\Omega_{ril}$</td>
<td>radial resistance to water transport from surface to axis of roots/mosses/mycorrhizae</td>
<td>MPa h m(^{-1})</td>
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<tr>
<td>$\Omega_{ril,l}$</td>
<td>radial resistance to water transport from soil to surface of roots/mosses/mycorrhizae</td>
<td>MPa h m(^{-1})</td>
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<tr>
<td>$\theta_{ei}$</td>
<td>soil water content</td>
<td>m(^3) m(^{-3})</td>
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<table>
<thead>
<tr>
<th>Symbol</th>
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<th>Unit</th>
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<tr>
<td>$\theta_{p}$</td>
<td>soil porosity</td>
<td>m$^3$ m$^{-3}$</td>
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<tr>
<td>$\theta_{P_{x,r}}$</td>
<td>root porosity</td>
<td>m$^3$ m$^{-3}$</td>
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<tr>
<td>$R_i$</td>
<td>Richardson number</td>
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<tr>
<td>$R_{n_{c_i}}$</td>
<td>canopy net radiation</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$r_{di}$</td>
<td>aerodynamic resistance to vapor flux from canopy</td>
<td>s m$^{-1}$</td>
</tr>
<tr>
<td>$r_{bd}$</td>
<td>radius of bole at ambient $\psi_{c_i}$</td>
<td>m</td>
</tr>
<tr>
<td>$r_{b_i}'$</td>
<td>radius of bole at $\psi_{c_i} = 0$ MPa</td>
<td>m</td>
</tr>
<tr>
<td>$r_{ci}$</td>
<td>canopy stomatal resistance to vapor flux</td>
<td>s m$^{-1}$</td>
</tr>
<tr>
<td>$r_{c_{max}}$</td>
<td>canopy cuticular resistance to vapor flux</td>
<td>s m$^{-1}$</td>
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<tr>
<td>$r_{c_{min}}$</td>
<td>minimum $r_{c_i}$ at $\psi_{c_i} = 0$ MPa</td>
<td>s m$^{-1}$</td>
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<tr>
<td>$r_{l,r,l,x}$</td>
<td>radius of primary ($x=1$) or secondary ($x=2$)</td>
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<tr>
<td>$r_{l,r,l,z}$</td>
<td>roots/mosses/mycorrhizae at ambient $\psi_{l_i,l,z}$</td>
<td>m</td>
</tr>
<tr>
<td>$r'_{l,r}$</td>
<td>radius of secondary roots/mosses/mycorrhizae at $\psi_{l_i,l,z} = 0$ MPa</td>
<td>m</td>
</tr>
<tr>
<td>$\rho_r$</td>
<td>root specific density</td>
<td>g C g FW$^{-1}$</td>
</tr>
<tr>
<td>$T_a$</td>
<td>air temperature</td>
<td>K</td>
</tr>
<tr>
<td>$T_c$</td>
<td>canopy temperature</td>
<td>K</td>
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<tr>
<td>$U_{wi}$</td>
<td>total water uptake from all rooted soil layers</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
</tr>
<tr>
<td>$U_{w_{i,x,l}}$</td>
<td>water uptake by root/moss/mycorrhizal surfaces in each soil layer</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
</tr>
</tbody>
</table>

(van Bavel and Hillel, 1976)
**\( u_a \)** wind speed measured at \( z_a \) m s\(^{-1}\)

**\( V'_{ci} \)** potential canopy CO\(_2\) fixation rate at \( \psi_{ci} = 0 \) MPa \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

**\( \nu_r \)** root specific volume \( \text{m}^3 \text{g FW}^{-1} \)

**\( X_{ci} \)** canopy capacitance \( \text{m}^3 \text{m}^{-2} \text{MPa}^{-1} \)

**\( \psi_{ci} \)** canopy water potential MPa

**\( \psi_{ci}' \)** \( \psi_{ci} \) + canopy gravitational potential MPa

**\( \psi_{ci}'' \)** canopy osmotic potential MPa

**\( \psi_{si} \)** soil water potential MPa

**\( \psi_{si}' \)** \( \psi_{si} \) + soil gravitational potential MPa

**\( \psi_{ti} \)** canopy turgor potential MPa 1.25 at \( \psi_c = 0 \)

**\( z_{bi} \)** length of bole from soil surface to top of canopy m

**\( z_{wi} \)** canopy zero-plane displacement height m

**\( z_l \)** depth of soil layer below surface m

**\( z_r \)** canopy surface roughness m

**\( z_u \)** height of wind speed measurement m

(Grant, 1998)

(Perrier, 1982)
Appendix C: Gross primary productivity and autotrophic respiration

**C₃ gross primary productivity**

\[ GPP = \sum_{i,j,k,l,m,n,o} (V_{c_{i,j,k,l,m,n,o}} = V_g_{i,j,k,l,m,n,o}) A_{i,j,k,l,m,n,o} \]

\[ V_{g_{i,j,k,l,m,n,o}} = (C_b - C_{i,j,k,l,m,n,o}) r_{i,j,k,l,m,n,o} \]

\[ V_{c_{i,j,k,l,m,n,o}} = \text{min} \left\{ V_{b_{i,j,k,l,m,n,o}}, V_{g_{i,j,k,l,m,n,o}} \right\} \]

\[ r_{i,j,k,l,m,n,o} = \left( r_{\text{mini},i,j,k,l,m,n,o} + \left( r_{\text{maxi},i,j,k,l,m,n,o} - r_{\text{mini},i,j,k,l,m,n,o} \right) e^{(-\beta \psi)} \right) \]

\[ V_{b_{i,j,k,l,m,n,o}} = V_{\text{bmax},i,j,k,l,m,n,o} \left( C_{c_{i,j,k,l,m,n,o}} - \Gamma_{i,j,k,l,m,n,o} \right) / \left( C_{c_{i,j,k,l,m,n,o}} + K_c \left( f_{\phi_{i,j,k,l,m,n,o}} \right) \right) \]

\[ V_{\text{bmax},i,j,k,l,m,n,o} = \left( \varepsilon_{I_{i,l,m,n,o}} + J_{\text{max},i,j,k,l,m,n,o} - \left( \varepsilon_{I_{i,l,m,n,o}} + J_{\text{max},i,j,k,l,m,n,o} \right)^2 - 4 \alpha \varepsilon_{I_{i,l,m,n,o}} J_{\text{max},i,k,l,m,n,o} \right) 0.5 \]

\[ J_{\text{max},i,j,k,l,m,n,o} = V_{j_{i,j,k,l,m,n,o}} F_{\text{chlorophyll}_{i,j,k,l,m,n,o}} A_{i,j,k,l,m,n,o} f_{\phi_{j,i}} \]

\[ f_{\phi_{i,j,k,l,m,n,o}} = \left( r_{\text{mini},i,j,k,l,m,n,o} / r_{i,j,k,l,m,n,o} \right)^{0.5} \]

solve for \( C_{i,j,k,l,m,n,o} \) at which \( V_{c_{i,j,k,l,m,n,o}} = V_{g_{i,j,k,l,m,n,o}} \) diffusion

\( C_b \) is leaf-level equivalent of \( r_c \) carboxylation

minimum \( r_i \) is driven by carboxylation

CO₂, water, temperature and nutrient constraints on \( V_b \)

water, temperature and nutrient constraints on \( V_j \)

non-stomatal effect related to stomatal effect
$$f_{oi} = \exp[B_{oi} - H_{oi}((RT)_{oi})] / \{1 + \exp[(H_{oi} - ST_{oi})/((RT)_{oi})] + \exp[(ST_{oi} - H_{oi})/((RT)_{oi})]\}$$

$$f_{oi} = \exp[B_{oi} - H_{oi}((RT)_{oi})] / \{1 + \exp[(H_{oi} - ST_{oi})/((RT)_{oi})] + \exp[(ST_{oi} - H_{oi})/((RT)_{oi})]\}$$

$$f_{ij} = \exp[B_{ij} - H_{ij}((RT)_{ij})] / \{1 + \exp[(H_{ij} - ST_{ij})/((RT)_{ij})] + \exp[(ST_{ij} - H_{ij})/((RT)_{ij})]\}$$

$$f_{iak} = \exp[B_{iak} - H_{iak}((RT)_{iak})]$$

$$f_{iak} = \exp[B_{iak} - H_{iak}((RT)_{iak})]$$

$$f_{cijkl} = \min\{\sigma_{cijkl} / (\sigma_{cijkl} + \sigma_{cijkl} / K_{C,N}), \sigma_{cijkl} / (\sigma_{cijkl} + \sigma_{cijkl} / K_{C,P})\}$$

$$\delta M_{i,j,k} / \delta t = \delta M_{i,j,k} / \delta t \min\{[N'_{\text{leat}} + (N_{\text{leat}} - N'_{\text{leat}}) f_{cik}] / N_{\text{prot}}, [P'_{\text{leat}} + (P_{\text{leat}} - P'_{\text{leat}}) f_{cik}] / P_{\text{prot}}\}$$

**Autotrophic respiration**

$$R_a = \Sigma_r \Sigma_i (R_{ci,j} + R_{si,j}) + \Sigma_r \Sigma_i \Sigma_z (R_{ci,r,t} + R_{si,r,t}) + E_{N, P} (U_{NH4,r,t} + U_{NO3,r,t} + U_{PO4,r,t})$$

$$R_{ci,j} = R_e \cdot \sigma_{cijkl} f_{uai}$$

$$R_{si,r,t} = R_e \cdot \sigma_{cijkl} f_{uai} (U_{O2,r,t} / U'_{O2,r,t})$$

$$U_{O2,r,t} = U'_{O2,r,t} [O2_{r,t}]/([O2_{r,t}] + K_{O2})$$

$$= U_{r,t} [O2_{r}] + 2\pi L_{i,r,t} D_{O2} ([O2_{r}] - [O2_{r,t}]) \ln\{(r_d + r_{i,r,t})/ r_{i,r,t}\}$$

$$+ 2\pi L_{i,r,t} D_{O2} ([O2_{r'}] - [O2_{r,t}]) \ln\{(r_d + r_{i,r,t})/ r_{i,r,t}\}$$

$$U'_{O2,r,t} = 2.67 R_{e,r,t}$$

$$R_{si,j} = \min\{0.0, R_{si,j} - R_{mi,j}\}$$

$$R_{mi,j} = \Sigma_z (N_{i,j,z} R_{ai} f_{umi})$$

$$R_{ai} = \max\{0.0, \min\{(R_{ci,j} - R_{mi,j}) \min\{0.0, \psi_{ai} - \psi'_{ai}\}\}$$

**Growth and senescence**

$$l_{i,j,c} = R_{ai} M_{i,Ni,j} / M_{i,Ri,j}$$

Arrhenius functions for carboxylation, oxygenation and electron transport temperature sensitivity of $K_{c,r}, K_{o}$ [SC10a]

product inhibition of $V_h$, $V_j$ from $\sigma_{N}$ and $\sigma_{P}$ vs. $\sigma_c$ in shoots leaf structural protein growth [SC10c]

total autotrophic respiration [SC13]

$O_2$ 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 [SC14b]

remobilization when $R_m > R_c$ [SC15]

maintenance respiration [SC16]

growth when $R_m < R_c$ [SC17]

senescence drives litterfall of non-remmobilizable material [SC18]
l_{i,j,N} = l_{i,j,C} N_{prot} (1.0 - X_{mx} f_{SN_i})

l_{i,j,P} = l_{i,j,C} P_{prot} (1.0 - X_{mx} f_{SP_i})

f_{SN_i} = \sigma_{SN_i}/(\sigma_{SN_i} + \sigma_{Ni}/K_{Ni})

f_{SP_i} = \sigma_{SP_i}/(\sigma_{SP_i} + \sigma_{Pi}/K_{Pi})

\delta M_{Rij}/\delta t = \Sigma_{j} [R_{grj} (1 - Y_{grj})/Y_{grj} - R_{dlj} - l_{ij,C}]

\delta M_{Rij}/\delta t = [R_{grj} (1 - Y_{grj})/Y_{grj} - R_{dlj} - l_{ij,C}]

\delta M_{Lij}/\delta t = \chi(M_{Lij}/\psi) / \sigma_{\delta t} \min\{1, \max\{0, \psi_t - \psi_i\}

\delta M_{Lij}/\delta t = \chi(M_{Lij}/\psi) / \sigma_{\delta t} \min\{1, \max\{0, \psi_t - \psi_i\}

f_{SW} = T_a \{\exp[B_v - H_{av}(RT_d)]/\{1 + \exp[(H_{ai} - ST_{ai})/(RT_d)] + \exp[(ST_{ai} - H_{ai})/(RT_d)]\}

f_{mil} = e^{-0.0811\cdot(T_{ci} - 298.15)}

**Root/moss/mycorrhizal nutrient uptake**

\[ U_{NH4,i} = \{U_{w,i}[\text{NH}_4^+] + 2\pi L_{r,i} D_{\text{NH}_4,\text{i}} ([\text{NH}_4^+] - [\text{NH}_4^+]) / \ln(d_{r,i}/r_{\text{r},i})\} \]

\[ = U^{1/2} \{U_{o2,i}/U^{1/2} A_{o2,i} ([\text{NH}_4^+] - [\text{NH}_4^+])/([\text{NH}_4^+] - [\text{NH}_4^+]) + K_{Ni} f_{SN_i}\} \]

\[ U_{NO3,i} = \{U_{w,i} [\text{NO}_3^-] + 2\pi L_{r,i} D_{\text{NO}_3,\text{i}} ([\text{NO}_3^-] - [\text{NO}_3^-]) / \ln(d_{r,i}/r_{\text{r},i})\} \]

\[ = U^{1/2} \{U_{o2,i}/U^{1/2} A_{o2,i} ([\text{NO}_3^-] - [\text{NO}_3^-])/([\text{NO}_3^-] - [\text{NO}_3^-]) + K_{No3} f_{SN_i}\} \]

\[ U_{PO4,i} = \{U_{w,i} [\text{H}_2\text{PO}_4^-] + 2\pi L_{r,i} D_{\text{PO}_4,\text{i}} ([\text{H}_2\text{PO}_4^-] - [\text{H}_2\text{PO}_4^-]) / \ln(d_{r,i}/r_{\text{r},i})\} \]

\[ = U^{1/2} \{U_{o2,i}/U^{1/2} A_{o2,i} ([\text{H}_2\text{PO}_4^-] - [\text{H}_2\text{PO}_4^-])/([\text{H}_2\text{PO}_4^-] - [\text{H}_2\text{PO}_4^-]) + K_{PO4} f_{SP_i}\} \]

**litterfall of N and P is driven by**

**branch growth driven by**

**root growth driven by**

**leaf growth driven by leaf mass**

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

**Arrhenius function for**

**temperature function for**

Root/moss/mycorrhizal N and P uptake from mass flow + diffusion coupled with active uptake of NH₄⁺, NO₃⁻ and H₂PO₄⁻ constrained by O₂ uptake, as for microbial N and P uptake [SA26]

product inhibition of UₙH₄, UₙO₃ and UₚO₄ determined by σₙ and σ₀ vs. σₐ in roots [SC23h]
## Definition of variables in Appendix C

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(i)</td>
<td>species or functional type: evergreen, coniferous, deciduous, annual, perennial, (C_3, C_4), monocot, dicot, legume etc.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(j)</td>
<td>branch or tiller</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(k)</td>
<td>Node</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(l)</td>
<td>soil or canopy layer</td>
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<td></td>
</tr>
<tr>
<td>(m)</td>
<td>leaf azimuth</td>
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</tr>
<tr>
<td>(n)</td>
<td>leaf inclination</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(o)</td>
<td>leaf exposure (sunlit vs. shaded)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(z)</td>
<td>organ including leaf, stem, root, moss mycorrhizae</td>
<td></td>
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</tbody>
</table>

### Subscripts

- \(i\): species or functional type
- \(j\): branch or tiller
- \(k\): Node
- \(l\): soil or canopy layer
- \(m\): leaf azimuth
- \(n\): leaf inclination
- \(o\): leaf exposure (sunlit vs. shaded)
- \(z\): organ

### Variables

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Value</th>
<th>Reference</th>
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<tbody>
<tr>
<td>(A)</td>
<td>leaf, root/moss/mycorrhizal surface area</td>
<td>m² m⁻²</td>
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<tr>
<td>(\beta)</td>
<td>shape parameter for stomatal effects on CO₂ diffusion and non-stomatal effects on carboxylation</td>
<td>MPa⁻¹</td>
<td>-5.0</td>
<td>(Grant and Flanagan, 2007)</td>
</tr>
<tr>
<td>(B)</td>
<td>parameter such that (f_i = 1.0) at (T_c = 298.15) K</td>
<td></td>
<td>17.533</td>
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<tr>
<td>(B_i)</td>
<td>parameter such that (f_{ij} = 1.0) at (T_c = 298.15) K</td>
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<td>17.363</td>
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<tr>
<td>(B_{ke})</td>
<td>parameter such that (f_{kce} = 1.0) at (T_c = 298.15) K</td>
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<td>(B_{ko})</td>
<td>parameter such that (f_{kco} = 1.0) at (T_c = 298.15) K</td>
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<td>8.067</td>
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<tr>
<td>(B_o)</td>
<td>parameter such that (f_{o} = 1.0) at (T_c = 298.15) K</td>
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<td>24.221</td>
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</table>
$B_v$ parameter such that $f_{vd} = 1.0$ at $T_c = 298.15$ K  

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>$C_b$</td>
<td>[CO$_2$] in canopy air</td>
<td>μmol mol$^{-1}$</td>
</tr>
<tr>
<td>$C_{c(b4)}$</td>
<td>[CO$_2$] in C$_4$ bundle sheath</td>
<td>μM</td>
</tr>
<tr>
<td>$C_{c(m4)}$</td>
<td>[CO$_2$] in C$<em>4$ mesophyll in equilibrium with $C</em>{i,j,k,l,m,n,o}$</td>
<td>μM</td>
</tr>
<tr>
<td>$C_c$</td>
<td>[CO$<em>2$] in canopy chloroplasts in equilibrium with $C</em>{i,j,k,l,m,n,o}$</td>
<td>μM</td>
</tr>
<tr>
<td>$C_{i(m4)}$</td>
<td>[CO$_2$] in C$<em>4$ mesophyll air when $\psi</em>{ci} = 0$</td>
<td>μmol mol$^{-1}$</td>
</tr>
<tr>
<td>$C_{i(m4)}$</td>
<td>[CO$_2$] in C$_4$ mesophyll air</td>
<td>μmol mol$^{-1}$</td>
</tr>
<tr>
<td>$C_{i,z,l}$</td>
<td>C content of leaf ($z=l$)</td>
<td>g C m$^{-2}$</td>
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<tr>
<td>$C_{i}'$</td>
<td>[CO$<em>2$] in canopy leaves when $\psi</em>{ci} = 0$</td>
<td>μmol mol$^{-1}$</td>
</tr>
<tr>
<td>$C_i$</td>
<td>[CO$_2$] in canopy leaves</td>
<td>μmol mol$^{-1}$</td>
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<tr>
<td>$D_{e\text{NH}_4}$</td>
<td>effective dispersivity-diffusivity of NH$_4^+$ during root/moss/mycorrhizal uptake</td>
<td>m$^2$ h$^{-1}$</td>
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<tr>
<td>$D_{e\text{NO}_3}$</td>
<td>effective dispersivity-diffusivity of NO$_3^-$ during root/moss/mycorrhizal uptake</td>
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<td>$D_{e\text{PO}_4}$</td>
<td>effective dispersivity-diffusivity of H$_2$PO$_4^-$ during root/moss/mycorrhizal uptake</td>
<td>m$^2$ h$^{-1}$</td>
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<td>$D_{O2}$</td>
<td>aqueous diffusivity of O$_2$ from root aerenchyma to root or mycorrhizal surfaces</td>
<td>m$^2$ h$^{-1}$</td>
</tr>
<tr>
<td>$D_{O2}$</td>
<td>aqueous diffusivity of O$_2$ from soil to root or mycorrhizal surfaces</td>
<td>m$^2$ h$^{-1}$</td>
</tr>
<tr>
<td>$d_{i,r,l}$</td>
<td>half distance between adjacent roots assumed equal to uptake path length</td>
<td>m</td>
</tr>
</tbody>
</table>

$0.45 \times C_b$

0.70 $\times C_b$ (Larcher, 2003)

$(\pi L_{a,z} / \Delta z)^{1/2}$ (Grant, 1998)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
<th>Value/Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{N,P}$</td>
<td>Energy cost of nutrient uptake</td>
<td>g C g $N^{-1}$ or $P^{-1}$</td>
<td>2.15 (Veen, 1981)</td>
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<tr>
<td>$f_{C_{(c3)}}$</td>
<td>$C_3$ product inhibition of RuBP carboxylation activity in $C_4$ bundle sheath or $C_3$ mesophyll</td>
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<tr>
<td>$f_{C_{(m4)}}$</td>
<td>$C_4$ product inhibition of PEP carboxylation activity in $C_4$ mesophyll</td>
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<tr>
<td>$F_{chl}$</td>
<td>Fraction of leaf protein in chlorophyll</td>
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<td>0.025</td>
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<tr>
<td>$f_{IC}$</td>
<td>N, P inhibition on carboxylation, leaf structural N, P growth</td>
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<td>$f_{IN}$</td>
<td>N inhibition on root/moss/mycorrhizal N uptake</td>
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<tr>
<td>$f_{IP}$</td>
<td>P inhibition on root/moss/mycorrhizal P uptake</td>
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<td>$F_{rubisco}$</td>
<td>Fraction of leaf protein in rubisco</td>
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<td>$f_{ta}$</td>
<td>Temperature effect on $R_{ai,j}$</td>
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<td>$f_{tb}$</td>
<td>Temperature effect on carboxylation</td>
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<td>$f_{tg}$</td>
<td>Temperature function for root/moss/mycorrhizal growth respiration</td>
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<td>$f_{tj}$</td>
<td>Temperature effect on electron transport</td>
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<tr>
<td>$f_{tkc}$</td>
<td>Temperature effect on $K_{ci}$</td>
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<td>(Bernacchi et al., 2001, 2003)</td>
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<tr>
<td>$f_{tko}$</td>
<td>Temperature effect on $K_{oi}$</td>
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<td>(Bernacchi et al., 2001, 2003)</td>
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<tr>
<td>$f_{tm}$</td>
<td>Temperature effect on $R_{mi,j}$</td>
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<td>Q_{10} = 2.25</td>
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<tr>
<td>$f_{to}$</td>
<td>Temperature effect on oxygenation</td>
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<td>$f_{tv}$</td>
<td>Temperature effect on carboxylation</td>
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<tr>
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<td>$f_{xN}$</td>
<td>fraction of $X_{mx} N$ translocated out of leaf or root/moss during senescence</td>
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<td>$f_{xP}$</td>
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<td>$f_{vni}$</td>
<td>non-stomatal water effect on carboxylation</td>
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<td>non-stomatal water effect on carboxylation</td>
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<td>$H_a$</td>
<td>energy of activation $\text{J} \text{mol}^{-1}$ $57.5 \times 10^3$</td>
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<td>$H_{aj}$</td>
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<td>$H_{ake}$</td>
<td>parameter for temperature sensitivity of $K_e$ $\text{J} \text{mol}^{-1}$ $55 \times 10^3$ (Bernacchi et al., 2001, 2003)</td>
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<td>$H_{ako}$</td>
<td>parameter for temperature sensitivity of $K_o$ $\text{J} \text{mol}^{-1}$ $20 \times 10^3$ (Bernacchi et al., 2001, 2003)</td>
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<td>$H_a o$</td>
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<td>$H_{av}$</td>
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<td>$H_{dh}$</td>
<td>energy of high temperature deactivation $\text{J} \text{mol}^{-1}$ $220 \times 10^3$</td>
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<td>$H_{dl}$</td>
<td>energy of low temperature deactivation $\text{J} \text{mol}^{-1}$ $198.0 \times 10^3$</td>
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<tr>
<td>$H_{dl}$</td>
<td>energy of low temperature deactivation $\text{J} \text{mol}^{-1}$ $190 \times 10^3$</td>
<td></td>
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<tr>
<td>$I$</td>
<td>Irradiance $\mu\text{mol m}^{-2} \text{s}^{-1}$</td>
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</tbody>
</table>
\[ J_{(b4)} \] electron transport rate in C\textsubscript{4} bundle sheath \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ J_{(m4)} \] electron transport rate in C\textsubscript{4} mesophyll \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ J \] electron transport rate in C\textsubscript{3} mesophyll \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ J_{\text{max}}' \] specific electron transport rate at non-limiting \( I \) and 25\textdegree C when \( \varphi_c = 0 \) and nutrients are nonlimiting \( \mu \text{mol g}^{-1} \text{s}^{-1} \) 400

\[ J_{\text{max}(b4)} \] electron transport rate in C\textsubscript{4} bundle sheath at non-limiting \( I \) \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ J_{\text{max}(m4)} \] electron transport rate in C\textsubscript{4} mesophyll at non-limiting \( I \) \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ J_{\text{max}} \] electron transport rate at non-limiting \( I, \varphi_c, \) temperature and N,P \( \mu \text{mol m}^{-2} \text{s}^{-1} \)

\[ K_{c(b4)} \] Michaelis-Menten constant for carboxylation in C\textsubscript{4} bundle sheath \( \mu \text{M} \) 30.0 at 25\textdegree C and zero O\textsubscript{2} (Lawlor, 1993)

\[ K_{c(m4)} \] Michaelis-Menten constant for carboxylation in C\textsubscript{4} mesophyll \( \mu \text{M} \) 3.0 at 25\textdegree C (Lawlor, 1993)

\[ K_c \] Michaelis-Menten constant for carboxylation at zero O\textsubscript{2} \( \mu \text{M} \) 12.5 at 25 \textdegree C (Farquhar et al., 1980)

\[ K_{i\text{C}_N} \] inhibition constant for growth in shoots from \( \sigma_C \) vs. \( \sigma_N \) \( \text{g C g N}^{-1} \) 100 (Grant, 1998)

\[ K_{i\text{C}_P} \] inhibition constant for growth in shoots from \( \sigma_C \) vs. \( \sigma_P \) \( \text{g C g P}^{-1} \) 1000 (Grant, 1998)

\[ K_{i\text{C4(b4)}} \] constant for CO\textsubscript{2} product inhibition of C\textsubscript{4} decarboxylation in C\textsubscript{4} bundle sheath \( \mu \text{M} \) 1000.0
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_{I_C(m4)}$</td>
<td>constant for C₄ product inhibition of PEP carboxylation activity in C₄ mesophyll</td>
<td>μM</td>
<td>$5 \times 10^6$</td>
</tr>
<tr>
<td>$K_{I_{lf}}$</td>
<td>constant for C₃ product inhibition of RuBP carboxylation activity in C₄ bundle sheath or C₃ mesophyll caused by $[\nu_{ilj}]$</td>
<td>g C g N⁻¹</td>
<td>100</td>
</tr>
<tr>
<td>$K_{I_{lf}}$</td>
<td>constant for C₃ product inhibition of RuBP carboxylation activity in C₄ bundle sheath or C₃ mesophyll caused by $[\alpha_{ilj}]$</td>
<td>g C g P⁻¹</td>
<td>1000</td>
</tr>
<tr>
<td>$K_{SC}$</td>
<td>inhibition constant for N uptake in roots/mosses from $\sigma_{C_{ilj}}$ vs. $\sigma_{N_{ij}}$</td>
<td>g N g C⁻¹</td>
<td>0.1</td>
</tr>
<tr>
<td>$K_{PC}$</td>
<td>inhibition constant for P uptake in roots/mosses from $\sigma_{C_{ilj}}$ vs. $\sigma_{P_{ilj}}$ roots</td>
<td>g P g C⁻¹</td>
<td>0.01</td>
</tr>
<tr>
<td>$K_{NH_4}$</td>
<td>M-M constant for NH₄⁺ uptake at root/moss/mycorrhizal surfaces</td>
<td>g N m⁻³</td>
<td>0.40</td>
</tr>
<tr>
<td>$K_{NO_3}$</td>
<td>M-M constant for NO₃⁻ uptake at root/moss/mycorrhizal surfaces</td>
<td>g N m⁻³</td>
<td>0.35</td>
</tr>
<tr>
<td>$K_{PO_4}$</td>
<td>M-M constant for H₂PO₄⁻ uptake root/moss/mycorrhizal surfaces</td>
<td>g P m⁻³</td>
<td>0.125</td>
</tr>
<tr>
<td>$K_{O_2}$</td>
<td>Michaelis-Menten constant for root or mycorrhizal O₂ uptake</td>
<td>g m⁻³</td>
<td>0.064</td>
</tr>
<tr>
<td>$K_o$</td>
<td>inhibition constant for O₂ in carboxylation</td>
<td>μM</td>
<td>500 at 25 ºC</td>
</tr>
<tr>
<td>$K_{AN}$</td>
<td>inhibition constant for remobilization of leaf or root/moss N during senescence</td>
<td>g N g C⁻¹</td>
<td>0.1</td>
</tr>
<tr>
<td>$K_{AP}$</td>
<td>inhibition constant for remobilization of leaf or root/moss P during senescence</td>
<td>g P g C⁻¹</td>
<td>0.01</td>
</tr>
</tbody>
</table>

$L$  root length

m m⁻²
\( \text{i}_C \) C litterfall from leaf or root/moss \( \text{g C m}^{-2} \text{ h}^{-1} \)

\( \text{i}_{N,P} \) N or P litterfall from leaf or root/moss \( \text{g C m}^{-2} \text{ h}^{-1} \)

\( \text{M}_B \) branch C phytomass \( \text{g C m}^{-2} \)

\( \text{M}_L \) leaf C phytomass \( \text{g C m}^{-2} \)

\( \text{M}_{L_{N,R}} \) non-remobilizable, remobilizable leaf C phytomass \( \text{g C m}^{-2} \)

\( \text{M}_R \) root C phytomass \( \text{g C m}^{-2} \)

\( \text{M}_{\text{prot}} \) leaf protein phytomass calculated from leaf N, P contents \( \text{g N m}^{-2} \)

\( \text{N}, \text{P} \) N or P content of organ \( \text{z} \) \( \text{g N m}^{-2} \)

\( \text{N}_{\text{prot}} \) N content of protein remobilized from leaf or root \( \text{g N C}^{-1} \)

\( \text{[NH}_4^+_{\text{r}}, \text{l}] \) concentration of \( \text{NH}_4^+ \) at root/moss/mycorrhizal surfaces \( \text{g N m}^{-3} \)

\( \text{[NH}_4^+_{\text{mn}} \) concentration of \( \text{NH}_4^+ \) at root/moss/mycorrhizal surfaces below which \( U_{\text{NH}_4} = 0 \) \( \text{g N m}^{-3} \)

\( \text{0.0125} \) (Barber and Silberbush, 1984)

\( \text{[NO}_3^-_{\text{r}}, \text{l}] \) concentration of \( \text{NO}_3^- \) at root/moss/mycorrhizal surfaces \( \text{g N m}^{-3} \)

\( \text{[NO}_3^-_{\text{mn}} \) concentration of \( \text{NO}_3^- \) at root/moss/mycorrhizal surfaces below which \( U_{\text{NO}_3} = 0 \) \( \text{g N m}^{-3} \)

\( \text{0.03} \) (Barber and Silberbush, 1984)

\( \text{[H}_2\text{PO}_4^-_{\text{r}}, \text{l}] \) concentration of \( \text{H}_2\text{PO}_4^- \) root/moss/mycorrhizal surfaces \( \text{g N m}^{-3} \)

\( \text{[H}_2\text{PO}_4^-_{\text{mn}} \) concentration of \( \text{H}_2\text{PO}_4^- \) root/moss/mycorrhizal surfaces below which \( U_{\text{PO}_4} = 0 \) \( \text{g N m}^{-3} \)

\( \text{0.002} \) (Barber and Silberbush, 1984)

\( \text{N}_{\text{leaf}} \) maximum leaf structural N content \( \text{g N g C}^{-1} \)

\( \text{0.10} \)

\( \text{N}_{\text{leaf}}' \) minimum leaf structural N content \( \text{g N g C}^{-1} \)

\( \text{0.33} \times \text{N}_{\text{leaf}} \)

\( \text{N}_{\text{lf}} \) total leaf N \( \text{g N m}^{-2} \text{ leaf} \)
\[ [N_{\text{chl(b4)}}]' \]
Ratio of chlorophyll N in C4 bundle sheath to total leaf N \( g \text{ N g}^{-1} \) 0.05

\[ [N_{\text{chl(m4)}}]' \]
Ratio of chlorophyll N in C4 mesophyll to total leaf N \( g \text{ N g}^{-1} \) 0.05

\[ [N_{\text{pep(m4)}}]' \]
Ratio of PEP carboxylase N in C4 mesophyll to total leaf N \( g \text{ N g}^{-1} \) 0.025

\[ [N_{\text{rub(b4)}}]' \]
Ratio of RuBP carboxylase N in C4 bundle sheath to total leaf N \( g \text{ N g}^{-1} \) 0.025

\( O_{2q} \)
Aqueous \( O_2 \) concentration in root or mycorrhizal aerenchyma \( g \text{ m}^{-3} \)

\( O_{2r} \)
Aqueous \( O_2 \) concentration at root or mycorrhizal surfaces \( g \text{ m}^{-3} \)

\( O_{2s} \)
Aqueous \( O_2 \) concentration in soil solution \( g \text{ m}^{-3} \)

\( O_c \)
\([O_2]\) in canopy chloroplasts in equilibrium with \( O_2 \) in atm. \( \mu \text{M} \)

\( P_{\text{leaf}} \)
Maximum leaf structural P content \( g \text{ P g}^{-1} \) 0.10

\( P'^{\text{leaf}} \)
Minimum leaf structural P content \( g \text{ P g}^{-1} \) 0.33 x \( P_{\text{leaf}} \)

\( P_{\text{prot}} \)
P content of protein remobilized from leaf or root \( g \text{ P C}^{-1} \) 0.04

\([\text{fr}]\)
Concentration of nonstructural root P uptake product in leaf \( g \text{ P g}^{-1} \)

\( \theta_P \)
Root or mycorrhizal porosity \( m^3 \text{ m}^{-3} \) 0.1 – 0.5

\( R \)
Gas constant \( J \text{ mol}^{-1} \text{ K}^{-1} \) 8.3143

\( R_a \)
Total autotrophic respiration \( g \text{ C m}^{-2} \text{ h}^{-1} \)

\( R_a' \)
\( R_a \) under nonlimiting \( O_2 \) \( g \text{ C m}^{-2} \text{ h}^{-1} \)

\( R_e' \)
Specific autotrophic respiration of \( \sigma_{C_{ij}} \) at \( T_{ci} = 25 \) °C \( g \text{ C g}^{-1} \text{ h}^{-1} \) 0.015
\( R_c \) autotrophic respiration of \( \sigma_{\text{Ci,j}} \) or \( \sigma_{\text{Ci,r,l}} \) g C m\(^2\) h\(^{-1}\)

\( R_g \) growth respiration g C m\(^2\) h\(^{-1}\)

\( r_l \) leaf stomatal resistance s m\(^{-1}\)

\( r_{\text{limaxi}} \) leaf cuticular resistance s m\(^{-1}\)

\( r_{\text{limini,j,k,l,m,n,o}} \) leaf stomatal resistance when \( \psi_{\text{ci}} = 0 \) s m\(^{-1}\)

\( r_{\text{ui,j,k,l,m,n,o}} \) leaf stomatal resistance s m\(^{-1}\)

\( r_{\text{maxi}} \) leaf cuticular resistance s m\(^{-1}\)

\( r_{\text{mini,j,k,l,m,n,o}} \) leaf stomatal resistance when \( \psi_{\text{ci}} = 0 \) s m\(^{-1}\)

\( R_{\text{u'}} \) specific maintenance respiration of \( \sigma_{\text{Ci,j}} \) at \( T_{\text{ci}} = 25^\circ\text{C} \) g C g N\(^{-1}\) h\(^{-1}\) 0.0115 (Barnes et al., 1997)

\( R_{\text{mi,j}} \) above-ground maintenance respiration g C m\(^2\) h\(^{-1}\)

\( r_{\text{qi,r,l}} \) radius of root aerenchyma m

\( r_{\text{ri,r,l}} \) root/moss/mycorrhizal radius m 1.0 \times 10^{-4} \text{ or } 5.0 \times 10^{-6}

\( R_{\text{sd,j}} \) respiration from remobilization of leaf C g C m\(^2\) h\(^{-1}\)

\( r_{\text{sd}} \) thickness of soil water films m

\( \rho_{r} \) dry matter content of root/moss biomass g g\(^{-1}\) 0.125 (Sharpe and DeMichele, 1977)

\( S \) change in entropy J mol\(^{-1}\) K\(^{-1}\) 710

\( \Delta S \) change in entropy J mol\(^{-1}\) K\(^{-1}\) 710

\( \sigma_{\text{C}} \) nonstructural C product of CO\(_2\) fixation g C g C\(^{-1}\)
\( \sigma_N \)  
nonstructural N product of root/moss/mycorrhizal uptake  
g N g C\(^{-1}\)

\( \sigma_P \)  
nonstructural P product of root/moss/mycorrhizal uptake  
g P g C\(^{-1}\)

\( T_c \)  
canopy temperature  
K

\( T_w \)  
canopy temperature  
°C

\( U_{NH_4,r,l} \)  
NH\(_4\)\(^+\) uptake by roots/mosses/mycorrhizae  
g N m\(^2\) h\(^{-1}\)

\( U'_NH_4 \)  
maximum \( U_{NH_4} \) at 25 °C and non-limiting NH\(_4\)\(^+\)  
g N m\(^2\) h\(^{-1}\)  
5.0 \times 10\(^{-3}\)  
(Barber and Silberbush, 1984)

\( U_{NO_3,r,l} \)  
NO\(_3\)\(^-\) uptake by roots/mosses/mycorrhizae  
g N m\(^2\) h\(^{-1}\)

\( U'_NO_3 \)  
maximum \( U_{NO_3} \) at 25 °C and non-limiting NO\(_3\)\(^-\)  
g N m\(^2\) h\(^{-1}\)  
5.0 \times 10\(^{-3}\)  
(Barber and Silberbush, 1984)

\( U_{PO_4,r,l} \)  
H\(_2\)PO\(_4\)\(^-\) uptake by roots/mosses/mycorrhizae  
g N m\(^2\) h\(^{-1}\)

\( U'_PO_4 \)  
maximum \( U_{PO_4} \) at 25 °C and non-limiting H\(_2\)PO\(_4\)  
g N m\(^2\) h\(^{-1}\)  
5.0 \times 10\(^{-3}\)  
(Barber and Silberbush, 1984)

\( U_{O_2,l,r} \)  
O\(_2\) uptake by roots and mycorrhizae under ambient O\(_2\)  
g O m\(^2\) h\(^{-1}\)

\( U'_O_2,l,r \)  
O\(_2\) uptake by roots and mycorrhizae under nonlimiting O\(_2\)  
g O m\(^2\) h\(^{-1}\)

\( U_{w,r,l} \)  
root/moss/mycorrhizal water uptake  
m\(^3\) m\(^{-2}\) h\(^{-1}\)

\( V_{b4b4,k,k} \)  
CO\(_2\) leakage from C\(_4\) bundle sheath to C\(_4\) mesophyll  
g C m\(^2\) h\(^{-1}\)

\( V_{b4} \)  
specific rubisco carboxylation at 25 °C  
\( \mu \)mol g\(^{-1}\) rubisco s\(^{-1}\)  
45  
(Farquhar et al., 1980)

\( V_{b4b4,k,k} \)  
CO\(_2\)-limited carboxylation rate in C\(_4\) bundle sheath  
\( \mu \)mol m\(^2\) s\(^{-1}\)

\( V_{b4m4,k,k,l,m,n,o} \)  
CO\(_2\)-limited carboxylation rate in C\(_4\) mesophyll  
\( \mu \)mol m\(^2\) s\(^{-1}\)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{bi,j,k,l,m,n,o}$</td>
<td>CO2-limited leaf carboxylation rate</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{max}(b4)}$</td>
<td>RuBP carboxylase specific activity in C$<em>4$ bundle sheath at 25°C when $\psi</em>{ci} = 0$ and nutrients are nonlimiting</td>
<td>$\mu$mol g$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{max}(b4),i,k}$</td>
<td>CO2-nonlimited carboxylation rate in C$_4$ bundle sheath</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{max}(m4)}$</td>
<td>PEP carboxylase specific activity in C$<em>4$ mesophyll at 25°C when $\psi</em>{ci} = 0$ and nutrients are nonlimiting</td>
<td>$\mu$mol g$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{max}(m4),i,j,k}$</td>
<td>CO2-nonlimited carboxylation rate in C$_4$ mesophyll</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{max},i,j,k}$</td>
<td>leaf carboxylation rate at non-limiting CO$<em>2$, $\psi</em>{ci}$, $T_c$ and N,P</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{c(b4),i,j,k,l,m,n,o}$</td>
<td>CO$_2$ fixation rate in C$_4$ bundle sheath</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{c(m4),i,j,k,l,m,n,o}$</td>
<td>CO$_2$ fixation rate in C$_4$ mesophyll</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{c(m4),i,j,k,l,m,n,o}$</td>
<td>CO$_2$ fixation rate in C$<em>4$ mesophyll when $\psi</em>{ci} = 0$ MPa</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{ci,j,k,l,m,n,o}$</td>
<td>leaf CO$_2$ fixation rate</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{c(i,j,k,l,m,n,o)}$</td>
<td>leaf CO$<em>2$ fixation rate when $\psi</em>{ci} = 0$</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{g(m4),i,j,k,l,m,n,o}$</td>
<td>CO$_2$ diffusion rate into C$_4$ mesophyll</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{g(i,j,k,l,m,n,o)}$</td>
<td>leaf CO$_2$ diffusion rate</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{j'}$</td>
<td>specific chlorophyll e$^-$ transfer at 25 °C</td>
<td>$\mu$mol g$^{-1}$ chlorophyll s$^{-1}$</td>
</tr>
<tr>
<td>$V_{j(b4),i,j,k,l,m,n,o}$</td>
<td>irradiance-limited carboxylation rate in C$_4$ bundle sheath</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>-------------------------------</td>
<td>--------------------------------------------------------------------------------------------------</td>
<td>--------------------</td>
</tr>
<tr>
<td>$V_{ij(m4),i,k,l,m,n,o}$</td>
<td>Irradiance-limited carboxylation rate in C$_4$ mesophyll</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{ij,k,l,m,n,o}$</td>
<td>Irradiance-limited leaf carboxylation rate</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_o'$</td>
<td>Specific rubisco oxygenation at 25 °C</td>
<td>$\mu$mol g$^{-1}$ rubisco s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{omax},i,k}$</td>
<td>Leaf oxygenation rate at non-limiting O$<em>2$, $\psi</em>{\text{ci}}$, $T_c$ and N,P</td>
<td>$\mu$mol m$^{-2}$ s$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{C4(b4),i,k}}$</td>
<td>Decarboxylation of C$_4$ fixation product in C$_4$ bundle sheath</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
</tr>
<tr>
<td>$V_{\text{C4(m4)}}$</td>
<td>Transfer of C$_4$ fixation product between C$_4$ mesophyll and bundle sheath</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
</tr>
<tr>
<td>$[\text{nlt}]$</td>
<td>Concentration of nonstructural root/moss/mycorrhizal N uptake product in leaf</td>
<td>g N g C$^{-1}$</td>
</tr>
<tr>
<td>$V_R$</td>
<td>Specific volume of root biomass</td>
<td>m$^3$ g$^{-1}$</td>
</tr>
<tr>
<td>$W_{\text{lf(b4)}}$</td>
<td>C$_4$ bundle sheath water content</td>
<td>g m$^{-2}$</td>
</tr>
<tr>
<td>$W_{\text{lf(m4)}}$</td>
<td>C$_4$ mesophyll water content</td>
<td>g m$^{-2}$</td>
</tr>
<tr>
<td>$X_{\text{mx}}$</td>
<td>Maximum fraction of remobilizable N or P translocated out of leaf or root during senescence</td>
<td>-</td>
</tr>
<tr>
<td>$Y_{(b4)}$</td>
<td>Carboxylation yield from electron transport in C$_4$ bundle sheath</td>
<td>$\mu$mol CO$_2$ $\mu$mol e$^{-1}$</td>
</tr>
<tr>
<td>$Y_{(m4)}$</td>
<td>Carboxylation yield from electron transport in C$_4$ mesophyll</td>
<td>$\mu$mol CO$_2$ $\mu$mol e$^{-1}$</td>
</tr>
<tr>
<td>$Y_{\text{g}}$</td>
<td>Fraction of $\sigma_{\text{C4,i,j}}$ used for growth expended as $R_{\text{g,z},i,j}$ by organ $z$</td>
<td>g C g C$^{-1}$</td>
</tr>
</tbody>
</table>

Source: (Farquhar et al., 1980)  
Source: (Kimmins, 2004)  
Source: (Kimmins, 2004)  
Source: (Waring and Running, 1998)
\( y \)  
plant population  
\( m^2 \)

\( Y \)  
carboxylation yield  
\( \mu \text{mol CO}_2 \mu \text{mol e}^{-1} \)

\( \Gamma \)  
CO\(_2\) compensation point  
\( \mu \text{M} \)

\( \Gamma_{(b4)} \)  
CO\(_2\) compensation point in C\(_4\) bundle sheath  
\( \mu \text{M} \)

\( \Gamma_{(m4)} \)  
CO\(_2\) compensation point in C\(_4\) mesophyll  
\( \mu \text{M} \)

\( \alpha \)  
shape parameter for response of \( J \) to \( I \)  
-  
0.7

\( \alpha \)  
shape parameter for response of \( J \) to \( I \)  
-  
0.75

\( \chi \)  
area:mass ratio of leaf growth  
\( m \text{ g}^{-3} \)  
0.0125  
(Grant and Hesketh, 1992)

\( \chi_{C4(b4)} \)  
non-structural C\(_4\) fixation product in C\(_4\) bundle sheath  
\( \mu \text{g C m}^{-2} \)

\( \chi_{C4(m4)} \)  
non-structural C\(_4\) fixation product in C\(_4\) mesophyll  
\( \mu \text{g C m}^{-2} \)

\( [\chi_{C3(b4)}] \)  
concentration of non-structural C\(_3\) fixation product in C\(_4\) bundle sheath  
\( \mu \text{g g}^{-1} \)

\( [\chi_{C4(m4)}] \)  
concentration of non-structural C\(_4\) fixation product in C\(_4\) mesophyll  
\( \mu \text{M} \)

\( \varepsilon \)  
quantum yield  
\( \mu \text{mol e}^{-} \mu \text{mol quanta}^{-1} \)  
0.45  
(Farquhar et al., 1980)

\( \varepsilon \)  
quantum yield  
\( \mu \text{mol e}^{-} \mu \text{mol quanta}^{-1} \)  
0.45  
(Farquhar et al., 1980)

\( \kappa_{C(b4)} \)  
conductance to CO\(_2\) leakage from C\(_4\) bundle sheath  
\( \text{h}^{-1} \)  
20

\( \psi_c \)  
canopy turgor potential  
MPa  
1.25 at \( \psi_c = 0 \)
Appendix D: Soil water, heat and gas fluxes

**Surface water flux**

\[
\frac{\Delta (d_w A)}{\Delta t} = \sum_i Q_{w, in} + \sum_i Q_{w, out} + P - E_{res} - E_{surf}; \text{ kinematic wave theory of overland flow} \tag{SD1}
\]

\[
Q_{w_i} = v_i (d_w - d_{sw}) L_i \tag{SD2}
\]

\[
v_i = \frac{R^{0.67} S_i^{0.5}}{z_r} \tag{SD3}
\]

\[
R = \frac{s d_{mw}}{s_r^2 + 1} \tag{SD4}
\]

\[
S_i = \frac{2 \text{abs}[(Z + d_{sw} + d_{mw})_i - (Z + d_{sw} + d_{mw})_d]}{L_x + L_{d_i}} \tag{SD5}
\]

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

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

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 h\(^{-1}\)); \( Z = \) surface elevation (m); \( d_{os} = \) 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 \((\psi_{res})\) 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.
residue (h m\(^{-1}\)); \(e_{\text{surf}}\) = vapour density at soil surface (g m\(^{-3}\)) at current soil surface water potential (\(\psi_{\text{surf}}\)) and temperature (\(T_{\text{surf}}\)); \(r_{\text{surf}}\) = boundary layer resistance to evaporation from soil surface (h m\(^{-1}\)); and \(r_{\text{surf}}\) = surface resistance to evaporation from soil surface (h m\(^{-1}\)).

### Sub-surface water flux

\[
\frac{\Delta \theta_{w}}{\Delta t} = \sum_{i}(Q_{w,\text{mat, in},i} + Q_{w,\text{mac, in},i} - Q_{w,\text{mat, out},i} - Q_{w,\text{mac, out},i}) + \sum_{j}(Q_{w,\text{b, mat, in},j} + Q_{w,\text{b, mac, in},j} - Q_{w,\text{b, mat, out},j} - Q_{w,\text{b, mac, out},j}) + Q_{f} - U_{w}
\]

; 3D continuity equation for water balance of each soil layer \[\text{SD8}\]

\[
Q_{w,\text{mat},i} = K'_{\text{mat},i}(\psi_{s,i} - \psi_{s,j})
\]

; soil matrix water flow \[\text{SD9}\]

\[
K'_{\text{mat},i} = \frac{2K_{\text{mat},i}K_{\text{mat},d,i}}{K_{\text{mat},i}L_{d,j} + K_{\text{mat},d,i}L_{s,i}}
\]

; when both the source and destination grid cells are either saturated or unsaturated (Richard’s equation) \[\text{SD10}\]

\[
K'_{\text{mat},i} = \frac{2K_{\text{mat},i}}{L_{d,i} + L_{s,i}}
\]

; when the source cell is saturated and the destination cell is unsaturated (Green-Ampt equation) \[\text{SD11}\]

\[
K'_{\text{mat},i} = \frac{2K_{\text{mat},d,i}}{L_{s,i} + L_{d,i}}
\]

; when the source cell is unsaturated and the destination cell is saturated (Green-Ampt equation) \[\text{SD12}\]

\[
K_{\text{mat},i} = K_{s,\text{mat}}\left(\frac{q - p + 1}{q}\right)^{1.33} \left[\frac{\sum_{p=1}^{q} 2p - 1}{\psi_{p}^{2}}\right] \left[\frac{\sum_{r=1}^{q} 2r + 1 - 2p}{\psi_{r}^{2}}\right]
\]

; Green and Corey (1971) model used in MCM simulation of ecosys \[\text{SD13}\]

\[
p = \text{Int} \left[q \left(\frac{\theta_{s} - \theta_{p}}{\theta_{s}}\right)\right] + 1
\]

; Green and Corey (1971) model used in MCM simulation of ecosys \[\text{SD14}\]
\[ n(k) = 1 + 0.001k \]  

\[ m(k) = 1 - \frac{1}{n(k)} \]  

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

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

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

\[ \theta_r(k) = \max \left[ 0, \frac{\theta_s - \theta_{r,\psi_{fc}} + \theta_{r,\psi_{wp}}}{S_{\phi,\text{con}}(k) - S_{\psi,\text{con}}(k)} \right] \]  

\[ \theta_{r,\psi_{fc,\text{con}}} = \theta_r(k) + \left[ \theta_s - \theta_r(k) \right] S_{\phi,\text{con}}(k) \quad \text{(van Genuchten 1980)} \]  

\[ \theta_{r,\psi_{wp,\text{con}}} = \theta_r(k) + \left[ \theta_s - \theta_r(k) \right] S_{\phi,\text{con}}(k) \quad \text{(van Genuchten 1980)} \]  

\[ K_{\text{mat}} = K_{s,\text{mat}} S_e^{-0.5} \left[ 1 - \left( 1 - S_e^\frac{1}{m} \right)^m \right]^2 \]  

where \( S_e = \frac{\theta - \theta_s}{\theta_s - \theta_r} = \left[ 1 + (\alpha \psi_{m})^{n} \right]^{-m} \); Mualem-van Genuchten model (Mualem, 1976; van Genuchten, 1980)  

used in VGM simulation of ecosys (Mezbahuddin et al., 2016)  

\[ K_{\text{mat}} = K_{s,\text{mat}} S_e^{-0.5} \left[ \frac{1 - \left( 1 - \left( S_e S_e^\frac{1}{m} \right)^m \right)^2}{1 - \left( 1 - S_e^\frac{1}{m} \right)^m} \right] \]  

where \( S_e = \frac{1}{S_e} \left[ 1 + (\alpha \psi_{m})^{n} \right]^{-m} \) and \( S_e = \left[ 1 + (\alpha \psi_{m})^{n} \right]^{-m} \); modified Mualem-van Genuchten model (Ippisch et al., 2006) used in VGM simulation of ecosys (Mezbahuddin et al., 2016)
\[ Q_{w,mac,i} = K'_{mac} \left( \psi_{g,i} - \psi_{g,d} \right) \]; soil macropore water flow

\[ K'_{mac} = \frac{2K_{mac,i}K_{mac,d}}{K_{mac,i}L_{d,i} + K_{mac,d}L_{s,i}} \]

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

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

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

\[ Q_{w,mat,j} = \frac{K_{b,mat,j} \left[ \psi'_{b} - \psi'_{s,j} + 0.01 \left( d_{z_b} - WTD_{x,j} \right) \right]}{L_{t,j}} \]; lateral discharge occurs when \( d_{z_b} < WTD_{x,j} \) and \( \psi'_{s,j} > \psi'_{b} + 0.01 \left( d_{z_b} - WTD_{x,j} \right) \) and lateral recharge occurs when \( d_{z_b} > WTD_{x,j} \)

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

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; \( \theta_{w}=\)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) (\( m^3 \ m^{-2} h^{-1} \)); \( U_r=\)total root water uptake flux (\( m^3 \ m^{-2} h^{-1} \)); \( K=\)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 \([1,2,3,\ldots, q]\); where \( q=\)total number of pore classes \((=100)\); \( \psi_{p}=\)matric potential of pore class \( p \); \( \psi_{r}=\)matric potential of pore class \( r \) (\( r=p\rightarrow q \)); \( n=\)van Genuchten parameter that describes the mean slope of the desorption curve or the range of pore size distribution; \( \alpha=\)the inverse of the pressure head at the air-entry value (i.e. \( \alpha=1/\)air entry potential) that governs the shape of van Genuchten desorption curve (\(-\)MPa\(^{-1}\)); \( k=\)number of iteration \((1,2,3,\ldots,19000)\); \( \psi_{in}=\)matric potential at inflection point (\(-\)MPa); \( S_{r,fc}=\)simulated relative degree of saturation at field capacity; \( \psi_{fc}=\)matric potential at field capacity (\(-\)MPa); \( S_{w,fc}=\)simulated relative degree of saturation at wilting point; \( \psi_{wp}=\)matric potential at wilting point (\(-\)MPa); \( \theta_{r}=\)residual soil water content (\( m^3 \ m^{-3} \)); \( \theta_{s,fc}=\)observed input for soil water content at field capacity (\( m^3 \ m^{-3} \)); \( \theta_{s,wp}=\)observed input...
for soil water content at wilting point (m$^3$ m$^{-3}$); $\theta_{v,wp}$ = simulated soil water content at wilting point (m$^3$ m$^{-3}$); $\theta_{v,fc}$ = simulated soil water content at field capacity (m$^3$ m$^{-3}$);

$\theta$ = ambient soil water content (m$^3$ m$^{-3}$); $\psi_m$ = matric potential as a function of $\theta$ (MPa); $\psi_e$ = matric potential very close to saturation (= 0.0001 MPa); $\psi_g$ = gravitational soil water potential (MPa); $N_{mac}$ = number of macropore channels (m$^{-2}$); $K_{*mac}$ = individual macropore hydraulic conductivity (m MPa$^{-1}$ h$^{-1}$ macropore channel$^{-1}$); $\eta$ = dynamic viscosity of water (MPa h); $\theta_{mac}$ = volumetric macropore fraction (m$^3$ m$^{-3}$);

$R_T$ = radius of a macropore channel (m); $\psi$ = 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 a particular grid cell

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); $\theta_g$ = current air-filled porosity of the layer immediately above the uppermost saturated layer (m$^3$ m$^{-3}$); and $\theta_g^*$ = 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

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

$$T_{frz} = \frac{-9.095895 \times 10^4}{\psi_m - 333} \text{ (for residue layer)} = \frac{-9.095895 \times 10^4}{\psi_m + \psi_e - 333} \text{ (for soil layers)}$$

$$T_{frz} = T_{frz} \text{ (for snowpack)}$$

$$G_{c,j} = \frac{2\zeta_{s, s} (T_s - T_g)}{L_i + L_d_i} + c_{w_s} T_w Q_w, \text{ (for soil layers)}$$

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\[
D_{\text{snowpack}} = \frac{V_{\text{sweq}} \rho_w + V_{\text{ice}} + V_{\text{water}}}{A_{\text{snowpack}}}
\]

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

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 (\(\text{Wm}^{-2}\)); \(LE\) = latent heat flux (\(\text{Wm}^{-2}\)); \(H\) = sensible heat flux (\(\text{Wm}^{-2}\)); \(G\) = conductive heat flux (\(\text{MJ m}^{-2} \text{h}^{-1}\)); \(L_f\) = latent heat of evaporation (=2460 \(\text{MJ m}^{-3}\)); \(\gamma_w\) = matric water potential of residue/soil layers (\(\text{MPa}\)); \(\gamma_o\) = osmotic potential of soil layers (\(\text{MPa}\)); \(T_{\text{frz}}\) = freezing temperature of free water (=273.15 K); \(\kappa\) = thermal conductivity (\(\text{MJ m}^{-1} \text{h}^{-1} \text{K}^{-1}\)); \(L\) = length of the residue layer/ a soil layer/ the snowpack (m); \(c_w\) = heat capacity of water (=4.19 \(\text{MJ m}^{-2} \text{K}^{-1}\)) ; \(Q_w\) = water flux (\(\text{m}^{-3} \text{m}^{-2} \text{h}^{-1}\)); \(D_{\text{snowpack}}\) = depth of snowpack (m); \(V_{\text{sweq}}\) = volume of snow water equivalent (m\(^3\)); \(\rho_w\) = density of water (=1 \(\text{Mg m}^{-3}\)); \(\rho_{\text{oldsnow}}\) = density of settled snow (\(\text{Mg m}^{-3}\)); \(V_{\text{ice}}\) = volume of ice in snowpack (m\(^3\)); \(V_{\text{water}}\) = volume of water in snowpack (m\(^3\)); \(A_{\text{snowpack}}\) = snowpack basal area (m\(^2\)); \(\rho_{\text{freshsnow}}\) = density of freshly fallen snow (=0.083 \(\text{Mg m}^{-3}\)); \(V_{\text{snow}}\) = volume of snow in the snowpack (m\(^3\)).

**Gas flux**

\[
Q_{\text{dry}} = \alpha_{a_s}D_{a_f} \left( S_{a_s} f_{a_s} \left[ \gamma_{a_s} \right]_s - \left[ \gamma_{a_s} \right]_s \right) ; \text{ volatilization-dissolution between aqueous and gaseous phases in soil}
\]

\[
Q_{\text{dry}} = \alpha_{a_s}D_{a_f} \left( S_{a_s} f_{a_s} \left[ \gamma_{a_s} \right]_s - \left[ \gamma_{a_s} \right]_s \right) ; \text{ volatilization-dissolution between aqueous and gaseous phases in roots}
\]

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

\[
Q_{\text{dry, i}} = -Q_{\text{w}} \left[ \gamma_{a_i} \right]_s + \frac{2D_{gry, i} \left[ \gamma_{a_i} \right]_s - \left[ \gamma_{a_i} \right]_d}{L_{s_i} + L_{d_i}} ; \text{ 3D convective-conductive gas flux between two adjacent grid cells}
\]
\[ Q_{gyr_{zz}} = \frac{D_{gyr_{zz}} \left[ \gamma_{gyr} \right]_d - \left[ \gamma_{gs} \right]}{\sum_{d_{z_{zz}}} L_{d_{zz}}}; \text{ convective-conductive gas flux between root and the atmosphere} \]  

\[ D_{gyr_{zz}} = \frac{D'_{gyr_{zz}} f_{g_{zs}} \left[ 0.5 \left( \theta_{gs} + \theta_{gd} \right) \right]^2}{\theta_{p_{gs}}^{0.67}}; \text{ 3D gaseous diffusivity between two adjacent grid cells as functions of air-filled porosities in those cells} \]  

\[ D_{gyr_{zz}} = \frac{D'_{gyr_{zz}} f_{g_{zs}} \theta_{gr_{zs}}^{1.33} A_{rs}}{A_{r=x,y}}; \text{ gaseous diffusivity as a function of air-filled porosity in the roots/mycorrhizae} \]

Where, subscripts \( i=x, y, z \); \( s=\text{source cell}, d=\text{destination cell}, surf=\text{soil surface layer}; Q_{gyr}=\text{volatilization – dissolution of gas} \gamma \text{ between aqueous and gaseous phases in soil (m}^2 \text{ h}^{-1}); \alpha_{gs}=\text{air-water interfacial area in soil (m}^2 \text{ m}^{-2}); D_{gyr}=\text{volatilization - dissolution transfer coefficient for gas} \gamma \text{ (m}^2 \text{ h}^{-1}); S'_{I} = \text{Ostwald solubility coefficient of gas} \gamma \text{ at 30°C (0.0293 for } \gamma=O_2 \text{)} (\text{Wilhelm et al., 1977}); f_{g_{I}} = \text{temperature dependence of } S'_{I} \text{ (Wilhelm et al., 1977)}; \]

\([\gamma_{gyr}]=\text{gaseous solubility coefficient of gas} \gamma \text{ in soil (g m}^{-3}); [\gamma_{gs}]=\text{aqueous concentration of gas} \gamma \text{ in soil (g m}^{-3}); Q_{gyr}=\text{volatilization – dissolution of gas} \gamma \text{ between aqueous and gaseous phases in root/moss (g m}^{-2} \text{ h}^{-1}); \alpha_{gs}=\text{air-water interfacial area in root/mycorrhizae (m}^2 \text{ m}^{-2})(\text{Skopp, 1985}); [\gamma_{gs}]=\text{gaseous concentration of gas} \gamma \text{ in root/mycorrhizae (g m}^{-3}); \gamma_{gs}=\text{gaseous concentration of gas} \gamma \text{ in root/moss/mycorrhizae (g m}^{-3}); Q_{gs}=\text{gaseous flux of gas} \gamma \text{ in soil (g m}^{-2} \text{ h}^{-1}); Q_{ws}=\text{sub-surface water flux (m}^2 \text{ h}^{-1}); D_{gyr}=\text{gaseous diffusivity of gas} \gamma \text{ in soil (m}^2 \text{ h}^{-1})(\text{Millington and Quirk, 1960}); L=\text{thickness of grid cells (m)}; Q_{gr}=\text{gaseous flux of gas} \gamma \text{ between root/mycorrhizae and the atmosphere (m}^2 \text{ h}^{-1}); D_{gr}=\text{gaseous diffusivity of gas} \gamma \text{ in root/mycorrhizae (m}^2 \text{ h}^{-1})(\text{Luxmoore et al., 1970a,b}); g_s = \text{boundary layer conductance (m h}^{-1}); [\gamma_s]=\text{atmospheric concentration of gas} \gamma \text{ (g m}^{-3}); D'_{gyr}=\text{diffusivity of gas} \gamma \text{ in air at } 0^\circ C (\text{m}^2 \text{ h}^{-1})(6.43 \times 10^{-2} \text{ m}^2 \text{ h}^{-1} \text{ for } \gamma=O_2) \text{ (Campbell, 1985)}; f_{g_{I}} = \text{temperature dependence of } D'_{gyr} \text{ (Campbell, 1985)}; \theta_{s}=\text{total porosity of soil (m}^3 \text{ m}^{-3}); \theta_{p} = \text{air-filled porosity (m}^3 \text{ m}^{-3}); A_r = \text{root cross-sectional area (m}^2); A = \text{area of landscape position (m}^2).
References


Table S1. Statistics from regressions between hourly modelled and gap-filled CO\textsubscript{2} fluxes from 2004-2009 at a Western Canadian fen peatland

### (a) Regressions of modelled vs. gap-filled ecosystem CO\textsubscript{2} fluxes over whole years of 2004-2008\textsuperscript{a}

<table>
<thead>
<tr>
<th>Year</th>
<th>Total annual precipitation (mm)</th>
<th>n</th>
<th>a</th>
<th>b</th>
<th>$R^2$</th>
<th>RMSE ((\mu\text{mol m}^{-2} \text{s}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>2004</td>
<td>553</td>
<td>3750</td>
<td>-0.13</td>
<td>1.20</td>
<td>0.89</td>
<td>0.64</td>
</tr>
<tr>
<td>2005</td>
<td>387</td>
<td>2807</td>
<td>-0.49</td>
<td>1.03</td>
<td>0.76</td>
<td>0.82</td>
</tr>
<tr>
<td>2006</td>
<td>465</td>
<td>2748</td>
<td>-0.48</td>
<td>1.15</td>
<td>0.81</td>
<td>0.58</td>
</tr>
<tr>
<td>2007</td>
<td>431</td>
<td>3375</td>
<td>-0.36</td>
<td>0.97</td>
<td>0.74</td>
<td>1.23</td>
</tr>
<tr>
<td>2008</td>
<td>494</td>
<td>2941</td>
<td>-0.54</td>
<td>1.05</td>
<td>0.79</td>
<td>0.95</td>
</tr>
</tbody>
</table>

### (b) Regressions of modelled vs. gap-filled net ecosystem CO\textsubscript{2} fluxes over growing seasons (May-August) of 2004-2009

<table>
<thead>
<tr>
<th>Year</th>
<th>Total growing season precipitation (mm)</th>
<th>n</th>
<th>a</th>
<th>b</th>
<th>$R^2$</th>
<th>RMSE ((\mu\text{mol m}^{-2} \text{s}^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>2004</td>
<td>287</td>
<td>837</td>
<td>-0.01</td>
<td>1.21</td>
<td>0.87</td>
<td>1.22</td>
</tr>
<tr>
<td>2005</td>
<td>276</td>
<td>680</td>
<td>-0.57</td>
<td>1.07</td>
<td>0.75</td>
<td>1.26</td>
</tr>
<tr>
<td>2006</td>
<td>253</td>
<td>773</td>
<td>-1.70</td>
<td>0.95</td>
<td>0.73</td>
<td>0.78</td>
</tr>
<tr>
<td>2007</td>
<td>237</td>
<td>1058</td>
<td>-0.51</td>
<td>0.98</td>
<td>0.76</td>
<td>1.88</td>
</tr>
<tr>
<td>2008</td>
<td>276</td>
<td>810</td>
<td>-1.04</td>
<td>1.02</td>
<td>0.79</td>
<td>1.62</td>
</tr>
<tr>
<td>2009</td>
<td>138</td>
<td>1010</td>
<td>-0.02</td>
<td>0.98</td>
<td>0.87</td>
<td>1.20</td>
</tr>
</tbody>
</table>

\(a, b\) from simple linear regressions of modelled on gap-filled, and $R^2 = \text{coefficient of determination}$; RMSE = root mean square for errors from simple linear regressions of gap-filled on simulated; \textsuperscript{a} whole year modelled vs. gap-filled CO\textsubscript{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.