

## Supplementary Material

### Introduction

*Ecosys* is an hourly time-step model with multiple canopy and soil layers that provide a framework for simulated plant and microbial populations to acquire, transform and exchange resources (energy, water, C, N and P). The model is constructed from algorithms representing basic physical, chemical and biological processes that determine process rates in plant and microbial populations interacting within complex biomes. These algorithms interact to simulate complex ecosystem behaviour across a wide range of spatial and biological scales. The model is designed to represent terrestrial ecosystems under range of natural and anthropogenic disturbances and environmental changes at patch (spatially homogenous one-dimensional) and landscape (spatially variable two- or three-dimensional) scales. A comprehensive description of *ecosys* with a detailed listing of inputs, outputs, governing equations, parameters, results and references can be found in Grant (2001). A more detailed description of model algorithms and parameters is given Supplements S1 to S8, with reference to equations and variable definitions in Tables S1 to S8. Variables in bold are model inputs with values given in the Definition of Variables associated with each table.

## **S1: Soil C, N and P Transformations**

### *Decomposition*

Organic transformations in *ecosys* occur in five organic matter–microbe complexes (coarse woody litter, fine non-woody litter, animal manure, particulate organic matter (POM), and humus) in each soil layer. Each complex consists of five organic states: solid organic matter  $S$ , dissolved organic matter  $Q$ , sorbed organic matter  $A$ , microbial biomass  $M$ , and microbial residues  $Z$ , among which C, N, and P are transformed. Organic matter in litter and manure complexes are partitioned from proximate analysis results into carbohydrate, protein, cellulose, and lignin components of differing vulnerability to hydrolysis. Organic matter in POM, humus, microbial biomass and microbial residues in all complexes are also partitioned into components of differing vulnerability to hydrolysis.

The rate at which each component of each organic state in each complex is hydrolyzed during decomposition is a first-order function of the decomposer biomass  $M$  of all heterotrophic microbial populations [A1]. Decomposer biomasses are redistributed among complexes from active biomasses according to biomass – substrate concentration differences (priming) [A3]. The rate at which each component is hydrolyzed is also a Monod function of substrate concentration [A3,A5], calculated from the fraction of substrate mass colonized by  $M$  [A4]. Hydrolysis rates are controlled by  $T_s$  through an Arrhenius function [A6] and by soil water content ( $\theta$ ) through its effect on aqueous microbial concentrations [ $M$ ] [A3,A5] in surface litter and in a spatially resolved soil profile.  $T_s$  and  $\theta$  are calculated from surface energy balances and from heat and water transfer schemes through canopy–snow–residue–soil profiles as described in *Energy Exchange* above. Release of N and P from hydrolysis of each component in each complex is determined by its N and P concentrations [A7] which are determined from those of the originating litterfall as described in *Autotrophic Respiration and Growth* above. Most non-lignin hydrolysis products are released as dissolved organic C, N and P (DOC, DON, and DOP) which are adsorbed or desorbed according to a power function of their soluble concentrations [A8 – A10].

### *Microbial Growth*

The DOC decomposition product is the substrate for heterotrophic respiration ( $R_h$ ) by all  $M$  in each substrate-microbe complex [A13]. Total  $R_h$  for all soil layers [A11] drives CO<sub>2</sub> emission from the soil surface through volatilization and diffusion.  $R_h$  may be constrained by microbial N or P concentrations,  $T_s$ , DOC and O<sub>2</sub> [A12 - A14]. O<sub>2</sub> uptake by  $M$  is driven by  $R_h$  [A16] and constrained by O<sub>2</sub> diffusivity to microbial surfaces [A17], as described for roots in *Autotrophic Respiration and Growth* above. Thus  $R_h$  is coupled to O<sub>2</sub> reduction by all aerobic  $M$  according to O<sub>2</sub> availability.  $R_h$  not coupled with O<sub>2</sub> reduction is coupled with the sequential

reduction of  $\text{NO}_3^-$ ,  $\text{NO}_2^-$ , and  $\text{N}_2\text{O}$  by heterotrophic denitrifiers, and with the reduction of organic C by fermenters and acetotrophic methanogens. In addition, autotrophic nitrifiers conduct  $\text{NH}_4^+$  and  $\text{NO}_2^-$  oxidation, and  $\text{NO}_2^-$  reduction, and autotrophic methanogens and methanotrophs conduct  $\text{CH}_4$  production and oxidation.

All microbial populations undergo maintenance respiration  $R_m$  [A18,A19], depending on microbial N and  $T_s$  as described earlier for plants.  $R_h$  in excess of  $R_m$  is used in growth respiration  $R_g$  [A20], the energy yield  $\Delta G$  of which drives growth in biomass  $M$  from DOC uptake according to the energy requirements of biosynthesis [A21, A22].  $R_m$  in excess of  $R_h$  causes microbial decay.  $M$  also undergoes first-order decay  $D_m$  [A23]. Internal recycling of microbial C, N and P decomposition products to nonstructural C, N and P pools during decay [A24] is modelled from nonstructural C,N,P ratios and from substrate concentration. Changes in  $M$  arise from differences between gains from DOC uptake and losses from  $R_m + R_g + D_m$  [A25].

#### *Microbial Nutrient Exchange*

During these changes, all microbial populations seek to maintain set minimum ratios of C:N or C:P in  $M$  by mineralizing or immobilizing  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ , and  $\text{H}_2\text{PO}_4^-$  [A26], thereby controlling solution  $[\text{NH}_4^+]$ ,  $[\text{NO}_3^-]$  and  $[\text{H}_2\text{PO}_4^-]$  that determine root and mycorrhizal uptake in *Nutrient Uptake and Translocation* above. If immobilization is inadequate to maintain these minimum ratios, then biomass C:N or C:P may rise, but  $R_h$  is constrained by N or P present in the lowest concentration with respect to that at the minimum ratio [A12]. Non-symbiotic heterotrophic diazotrophs can also fix aqueous  $\text{N}_2$  [A27] to the extent that immobilization is inadequate to maintain their set minimum C:N, but at an additional respiration cost [A28]. Changes in microbial N and P arise from DON and DOP uptake plus  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ , and  $\text{H}_2\text{PO}_4^-$  immobilization and  $\text{N}_2$  fixation, less  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ , and  $\text{H}_2\text{PO}_4^-$  mineralization and microbial N and P decomposition [A29].

#### *Humification*

C, N and P decomposition products in each organic matter–microbe complex are gradually stabilized into more recalcitrant organic forms with lower C:N and C:P ratios. Products from lignin hydrolysis [A1,A7] combine with some of the products from protein and carbohydrate hydrolysis in the litterfall and manure complexes and are transferred to the POM complex [A31–A34]. Microbial decomposition products [A23, A24] from all complexes are partitioned between the humus complex and microbial residues in the originating complex according to soil clay content [A35, A36].

**Table S1: Microbial C, N and P Transformations**

*Decomposition*

$D_{Si,j,l,C} = D'_{Si,j,l,C} M_{i,d,l,C} f_{tg,l} (S_{i,l,C} / G_{i,l,C})$	decomposition of litter, POC, humus	[A1a]
$D_{Zi,j,l,C} = D'_{Zi,j,l,C} M_{i,d,l,C} f_{tg,l} (Z_{i,l,C} / G_{i,l,C})$	decomposition of microbial residues	[A1b]
$D_{Ai,l,C} = D'_{Ai,l,C} M_{i,d,l,C} f_{tg,l} (A_{i,l,C} / G_{i,l,C})$	decomposition of adsorbed SOC	[A1c]
$S_{i,l,C} = \sum_j S_{i,j,l,C}$	total C in all kinetic components of litter, POC, humus	[A2a]
$Z_{i,l,C} = \sum_j Z_{i,j,l,C}$	total C in all kinetic components of microbial residues	[A2b]
$G_{i,l,C} = S_{i,l,C} + Z_{i,l,C} + A_{i,l,C}$	total C in substrate-microbe complexes	[A2c]
$M_{i,d,l,C} = M_{i,a,l,C} + \mathbf{q}_m (M_{i,a,l,C} G_{i,x,l,C} - M_{i,x,a,l,C} G_{i,l,C}) / (G_{i,x,l,C} + G_{i,l,C})$	redistribution of active microbial biomass populations from each substrate-microbe complex $i$ to other substrate-microbe complexes $ix$ according to concentration differences (priming)	[A3a]
$M_{i,a,l,C} = \sum_n M_{i,n,a,l,C}$	substrate and water constraint on $D$ from colonized litter, POC and humus, microbial residues and adsorbed SOC	[A3b]
$D'_{Si,j,l,C} = \{D_{Sj,C} [S_{i,j,l,C}]\} / \{[S_{i,j,l,C}] + K_{mD} (1.0 + [\sum M_{i,d,l,C}] / K_{iD})\}$	colonized litter increases with microbial growth into uncolonized litter	[A4a]
$D'_{Zi,j,l,C} = \{D_{Zj,C} [Z_{i,j,l,C}]\} / \{[Z_{i,j,l,C}] + K_{mD} (1.0 + [M_{i,d,l,C}] / K_{iD})\}$	Arrhenius function for $D$ and $R_h$	[A4b]
$D'_{Ai,l,C} = \{D_{Aj,C} [A_{i,l,C}]\} / \{[A_{i,l,C}] + K_{mD} (1.0 + [M_{i,d,l,C}] / K_{iD})\}$		[A4c]
$\delta S_{i,j,k,l,C} / \delta t = \beta \sum_n (U_{i,n,l,C} - R_{hi,n,l}) (S'_{i,j,k,l,C} / S'_{i,j,l,C}) \{(S'_{i,j,l,C} / S_{i,j,l,C}) / (S'_{i,j,l,C} / S_{i,j,l,C} + K_{is})\}$		[A5]
$f_{tg,l} = T_{sl} \{e^{[B - H_a / (R T_{sl})]}\} / \{1 + e^{[(H_{dl} - ST_{sl}) / (R T_{sl})]} + e^{[(ST_{sl} - H_{dh}) / (R T_{sl})]}\}$		[A6]

$D_{Si,j,l,N,P} = D_{Si,j,l,C} (S_{i,j,l,N,P} / S_{i,j,l,C})$	decomposition of N and P are driven by that of C in litter, POC, humus, microbial residues and adsorbed SOC	[A7a]
$D_{Zi,j,l,N,P} = D_{Zi,j,l,C} (Z_{i,j,l,N,P} / Z_{i,j,l,C})$		[A7b]
$D_{Ai,l,N,P} = D_{Ai,l,C} (A_{i,l,N,P} / A_{i,l,C})$		[A7c]
$Y_{i,l,C} = k_{ts} (G_{i,l,C} F_s [Q_{i,l,C}]^b - V_{i,l,C})$	Freundlich sorption of DOC	[A8]
$Y_{i,l,N,P} = Y_{i,l,C} (Q_{i,l,N,P} / Q_{i,l,C})$	$(Y_{i,l,C} > 0)$ adsorption of DON, DOP $(Y_{i,l,C} < 0)$ desorption of DON, DOP	[A9]
$Y_{i,l,N,P} = Y_{i,l,C} (V_{i,l,N,P} / V_{i,l,C})$		[A10]

### Microbial Growth

$R_h = \sum_i \sum_n \sum_l R_{hi,n,l}$	total heterotrophic respiration	[A11]
$R_{hi,n,l} = R'_{hn} \min\{C_{Ni,n,l,a} / C_{Nj}, C_{Pi,n,l,a} / C_{Pj}\}$	$R_h$ constrained by microbial N, P	[A12]
$R'_{i,n,l} = M_{i,n,a,l,C} \{R_{hi,n,l} [Q_{i,l,C}] / (K_m Q_C + [Q_{i,l,C}])\} f_{tg,l} f_{\psi gl}$	$R_h$ constrained by substrate DOC, $T_s$ and $\psi$	[A13]
$R_{hi,n,l} = R'_{i,n,l} (U_{O2i,n,l} / U'_{O2i,n,l})$	$R_h$ constrained by $O_2$	[A14]
$f_{\psi gl} = e^{(\sigma \psi_s l)}$	$\psi_s$ constraints on microbial growth	[A15]
$U'_{O2i,n,l} = 2.67 R'_{i,n,l}$	$O_2$ demand driven by potential $R_h$	[A16]
$U_{O2i,n,l} = U'_{O2i,n,l} [O_{2mi,n,l}] / ([O_{2mi,n,l}] + K_{O_2})$	active uptake coupled with radial diffusion of $O_2$	[A17a]
$= 4 \pi n M_{i,n,a,l,C} D_{SO2l} [r_m r_{wl} / (r_{wl} - r_m)] ([O_{2sl}] - [O_{2mi,n,l}])$		[A17b]
$R_{mi,n,j,l} = R_m M_{i,n,j,l,N} f_{tm,l}$	maintenanace respiration	[A18]
$f_{tm,l} = e^{[y (T_{sl} - 298.16)]}$	temperature sensitivity of $R_m$	[A19]
$R_{gi,n,l} = R_{hi,n,l} - \sum_j R_{mi,n,j,l}$	growth respiration	[A20]
$Y_g = -\Delta G_x / E_m$	growth yield of aerobic heterotrophs	[A21a]

$U_{i,n,lC} = \min (R_{hi,n,l}, \Sigma_j R_{mi,n,j,l}) + R_{gi,n,l}(1 + Y_g)$	DOC uptake driven by $R_g$	[A21b]
$U_{i,n,lN,P} = U_{i,n,l} Q_{i,l,N,P} / Q_{i,l,C}$	DON, DOP uptake driven by $U_{i,n,lC}$	[A22]
$D_{Mi,n,j,l,C} = D_{Mi,j} M_{i,n,j,C} (1.0 - (X_{Cmn} + (X_{Cmx} - X_{Cmn}) f_{\lambda,Ci,n,j,l}))$	decay of microbial C less internal recycling	[A23a]
$D_{Mi,n,j,l,N,P} = D_{Mi,j} M_{i,n,j,l,N,P} (1.0 - X_{N,P} f_{\lambda,N,Pi,n,j,l})$	decay of microbial N, P less internal recycling	[A23b]
$f_{\lambda,Ci,n,j,l} = \min \{M_{i,n,n,l,N} / (M_{i,n,n,l,N} + M_{i,n,n,l,C} K_{\lambda N}), M_{i,n,n,l,P} + M_{i,n,n,l,C} K_{\lambda P}\} (1.0 - [Q_{i,l,C}] / (K_{mQ} + [Q_{i,l,C}]))$	internal C,N,P recycling determined by nonstructural C,N,P ratios and by substrate concentration	[A24a]
$f_{\lambda,N,Pi,n,j,l} = M_{i,n,n,l,C} / (M_{i,n,n,l,C} + M_{i,n,n,l,N,P} / K_{\lambda N,P})$	[A24b]	
$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,lC} - F_j R_{hi,n,l} - D_{Mi,n,j,l,C}$	$[R_{hi,n,l} > R_{mi,n,j,l}]$ microbial growth	[A25a]
$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,lC} - R_{mi,n,j,l} - D_{Mi,n,j,l,C}$	$[R_{hi,n,l} < R_{mi,n,j,l}]$ microbial senescence	[A25b]

### Microbial Nutrient Exchange

$U_{NH4i,n,j,l} = (M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N})$	$U_{NH4} < 0$	net mineralization	[A26a]
$U_{NH4i,n,j,l} = \min \{(M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N}), U'_{NH4} a_{i,n,j,l} ([NH_4^+_{i,n,j,l}] - [NH_4^+_{mn}]) / ([NH_4^+_{i,n,j,l}] - [NH_4^+_{mn}] + K_{NH4})\}$	$U_{NH4} > 0$	net immobilization	[A26b]
$U_{NO3i,n,j,l} = \min \{(M_{i,n,j,l,C} C_{Nj} - (M_{i,n,j,l,N} + U_{NH4i,n,j,l})), U'_{NO3} a_{i,n,j,l} ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}]) / ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}] + K_{NO3})\}$	$U_{NO3} > 0$	net immobilization	[A26c]
$U_{PO4i,n,j,l} = (M_{i,n,j,l,C} C_{Pj} - M_{i,n,j,l,P})$	$U_{PO4} < 0$	net mineralization	[A26d]
$U_{PO4i,n,j,l} = \min \{(M_{i,n,j,l,C} C_{Pj} - M_{i,n,j,l,P}), U'_{PO4} A_{i,n,j,l} ([H_2PO_4^-_{i,n,j,l}] - [H_2PO_4^-_{mn}]) / ([H_2PO_4^-_{i,n,j,l}] - [H_2PO_4^-_{mn}] + K_{PO4})\}$	$U_{PO4} > 0$	net immobilization	[A26e]
$\Phi_{i,n=f,j,l} = \max \{0, M_{i,n=f,j,l,C} C_{Nj} - M_{i,n=f,j,l,N} - \max \{0, U_{i,n=f,j,l,N}\}\}$	$N_2$ fixation driven by N deficit of diazotrophic population	[A27]	
$R_{\phi i,n=f,j,l} = E_{\phi} \Phi_{i,n=f,j,l}$	respiration needed to drive $N_2$ fixation	[A28]	

$$\delta M_{i,n,j,l,N} / \delta t = F_j U_{i,n,l,N} + U_{\text{NH}_4i,n,j,l} + U_{\text{NO}_3i,n,j,l} + \Phi_{i,n=f,j,l} - D_{Mi,n,j,l,N} \quad \text{growth vs. losses of microbial N, P} \quad [\text{A29a}]$$

$$\delta M_{i,n,j,l,P} / \delta t = F_j U_{i,n,l,P} + U_{\text{PO}_4i,n,j,l} - D_{Mi,n,j,l,P} \quad [\text{A29b}]$$

$$M_{i,n,a,l,C} = M_{i,n,j=\text{labile},l,C} + M_{i,n,j=\text{resistant},l,C} F_r / F_1 \quad \text{active microbial biomass} \quad [\text{A30a}]$$

calculated from labile fraction

### Humification

$$H_{Si,j=\text{lignin},l,C} = D_{Si,j=\text{lignin},l,C} \quad \text{decomposition products of litter} \quad [\text{A31}]$$

$$H_{Si,j=\text{lignin},l,N,P} = D_{Si,j=\text{lignin},l,N,P} \quad \text{substrate added to POC depending} \quad [\text{A32}]$$

on lignin

$$H_{Si,j \neq \text{lignin},l,C} = H_{Si,j=\text{lignin},l,C} \mathbf{L}_{hj} \quad [\text{A33}]$$

$$H_{Si,j \neq \text{lignin},l,N,P} = H_{Si,j \neq \text{lignin},l,C} S_{i,l,N,P} / S_{i,l,C} \quad [\text{A34}]$$

$$H_{Mi,n,j,l,C} = D_{Mi,n,j,l,C} \mathbf{F}_h \quad \text{fraction of microbial decay} \quad [\text{A35}]$$

products added to humus

$$H_{Mi,n,j,l,N,P} = D_{Mi,n,j,l,N,P} \mathbf{F}_h \quad [\text{A36}]$$

$$\mathbf{F}_h = 0.167 + 0.167 F_{\text{clay}} \quad \text{fraction of } D_M \text{ added to humus} \quad [\text{A37}]$$

depends on clay

$$H_{Zi,n,j,l,C} = D_{Mi,n,j,l,C} - H_{Mi,n,j,l,C} \quad \text{remainder of microbial decay} \quad [\text{A38}]$$

$$H_{Zi,n,j,l,N,P} = D_{Mi,n,j,l,N,P} - H_{Mi,n,j,l,N,P} \quad \text{products added to microbial} \quad [\text{A39}]$$

residues

## Definition of Variables in Table S1

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus				
<i>j</i>	kinetic component: labile <i>l</i> , resistant <i>r</i> , active <i>a</i> , nonstructural <i>n</i>				
<i>l</i>	soil or litter layer				
<i>n</i>	microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)				
<i>variables</i>					
$A_{i,l,C}$	mass of adsorbed SOC	$\text{g C m}^{-2}$	[A1c,A2c]		
$[A_{i,l,C}]$	concentration of adsorbed SOC in soil	$\text{g C Mg}^{-1}$	[A4c]		
$a$	microbial surface area	$\text{m}^2 \text{ m}^{-2}$	[A26]		
$B$	parameter such that $f_{tg} = 1.0$ at $T_l = 298.15 \text{ K}$		[A6]	26.235	
$b$	Freundlich exponent for sorption isotherm		[A8]	0.85	Grant et al. (1993a,b)
$\beta$	specific colonization rate of uncolonized substrate	-	[A5]	2.5	Grant et al. (2010)
$C_{N,Pi,n,a,l}$	ratio of $M_{i,n,a,N,p}$ to $M_{i,n,a,C}$	$\text{g N or P g C}^{-1}$	[A12]		

$C_{N,P_j}$	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 <sup>-1</sup>	[A12,A26,A27]	0.22 and 0.13 (N), 0.022 and 0.013 (P) for $j$ = labile and resistant, respectively	Grant et al. (1993a,b)
$D_{A,i,l,C}$	decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ producing $Q$ in [A13]	g C m <sup>-2</sup> h <sup>-1</sup>	[A1c,A7c,A31c]		
$D_{A,j,C}$	specific decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ at 25°C and saturating [ $A_{i,l,C}$ ]	g C g C <sup>-1</sup> h <sup>-1</sup>	[A4c]	0.025	Grant et al. (1993a,b)
$D_{A,i,j,l,N,P}$	decomposition rate of $A_{i,l,N,P}$ by $M_{i,d,l,C}$	g N or P m <sup>-2</sup> h <sup>-1</sup>	[A7c]		
$D'_{A,i,j,l,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C <sup>-1</sup> h <sup>-1</sup>	[A1a,A4c]		
$D_{M,i,j}$	specific decomposition rate of $M_{i,n,j}$ at 30°C	g C g C <sup>-1</sup> h <sup>-1</sup>	[A23a,b]	2.0 x 10 <sup>-3</sup> and 1.0 x 10 <sup>-4</sup> for $j$ = labile and resistant, respectively	Grant et al. (1993a,b)
$D_{M,i,n,j,l,C}$	decomposition rate of $M_{i,n,j,l,C}$	g C m <sup>-2</sup> h <sup>-1</sup>	[A23a,A25,A35, A38]		
$D_{M,i,n,j,l,N,P}$	decomposition rate of $M_{i,n,j,l,N,P}$	g N or P m <sup>-2</sup> h <sup>-1</sup>	[A23b,A29,A39]		
$D_{S,i,j,l,C}$	decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing $Q$ in [A13]	g C m <sup>-2</sup> h <sup>-1</sup>	[A1a,A7a,A31a]		
$D_{S,j,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating [ $S_{i,l,C}$ ]	g C g C <sup>-1</sup> h <sup>-1</sup>	[A4a]	1.0, 1.0, 0.15, and 0.025 for $j$ = protein, carbohydrate, cellulose, and lignin, 0.009 for POC, and 0.009 and 0.003 for active and passive humus.	Grant et al. (1993a,b)
$D_{S,i,j,l,N,P}$	decomposition rate of $S_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m <sup>-2</sup> h <sup>-1</sup>	[A7a, A32]		

$D'_{S,i,j,l,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A1a,A4a]		
$D_{sO2l}$	aqueous dispersivity–diffusivity of O <sub>2</sub> during microbial uptake in soil	$\text{m}^2 \text{ h}^{-1}$	[A17]		
$D_{Z,i,j,l,C}$	decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing $Q$ in [A13]	$\text{g C m}^{-2} \text{ h}^{-1}$	[A1b,A7b]		
$D_{Z,i,j,N,P}$	decomposition rate of $Z_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A7b]		
$D_{Z,j,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating $[Z_{i,l,C}]$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A4b]	0.25 and 0.05 for $j = \text{labile and}$ resistant biomass	Grant et al. (1993a,b)
$D'_{Z,i,j,l,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A1b,A4b]		
$\Delta G_x$	energy yield of C oxidation with different reductants $x$	$\text{kJ g C}^{-1}$	[A21]	37.5 ( $x = \text{O}_2$ ), 4.43 ( $x = \text{DOC}$ )	
$E_m$	energy requirement for growth of $M_{i,n,a,l}$	$\text{kJ g C}^{-1}$	[A21]	25	
$E_\phi$	energy requirement for non-symbiotic N <sub>2</sub> fixation by heterotrophic diazotrophs ( $n = f$ )	$\text{g C g N}^{-1}$	[A28]	5	Waring and Running (1998)
$F_{\text{clay}}$	fraction of mineral soil as clay	$\text{Mg Mg}^{-1}$	[A37]		
$F_h$	fraction of products from microbial decomposition that are humified (function of clay content)		[A35, A37]		Sørenson (1981)
$F_l$	fraction of microbial growth allocated to labile component $M_{i,n,l}$		[A25,A29,A30]	0.55	Grant et al. (1993a,b)
$F_r$	fraction of microbial growth allocated to resistant component $M_{i,n,r}$		[A25,A29,A30]	0.45	Grant et al. (1993a,b)
$F_s$	equilibrium ratio between $Q_{i,l,C}$ and $H_{i,l,C}$		[A8]		
$f_{\lambda C,i,n,j,l}$	fraction of C recycled to nonstructural pool during decomposition	-	[A23a,A24a]		
$f_{\lambda N,P,i,n,j,l}$	fraction of N or P recycled to nonstructural pool during decomposition	-	[A23b,A24b]		
$f_{\text{gl}}$	temperature function for microbial growth respiration	dimensionless	[A1,A6,A13]		
$f_{\text{tm}}$	temperature function for maintenance respiration	dimensionless	[A18,A19]		

$f_{\psi gl}$	soil water potential function for microbial, root or mycorrhizal growth respiration	dimensionless	[A13,A15]	Pirt (1975)
$\Phi_{i,n=f,j,l}$	non-symbiotic $\text{N}_2$ fixation by heterotrophic diazotrophs ( $n=f$ )	$\text{g N m}^{-2} \text{ h}^{-1}$	[A27,A28,A29]	
$G_{i,l,C}$	total C in substrate-microbe complex	$\text{g C Mg}^{-1}$	[A1,A2c,A3a,A8, A37]	
$[\text{H}_2\text{PO}_4^-]$	concentration of $\text{H}_2\text{PO}_4^-$ in soil solution	$\text{g P m}^{-3}$	[A26]	
$H_a$	energy of activation	$\text{J mol}^{-1}$	[A6,C10]	$65 \times 10^3$
$H_{dh}$	energy of high temperature deactivation	$\text{J mol}^{-1}$	[A6,C10]	$225 \times 10^3$
$H_{dl}$	energy of low temperature deactivation	$\text{J mol}^{-1}$	[A6,C10]	$195 \times 10^3$
$H_{Mi,n,j,l,C}$	transfer of microbial C decomposition products to humus	$\text{g C m m}^{-2} \text{ h}^{-1}$	[A35,A36,A38]	
$H_{Mi,n,j,l,N,P}$	transfer of microbial N or P decomposition products to humus	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A36,A39]	
$H_{Si,j,l,C}$	transfer of C hydrolysis products to particulate OM	$\text{g C m}^{-2} \text{ h}^{-1}$	[A31,A32,A33, A34]	
$H_{Si,j,l,N,P}$	transfer of N or P hydrolysis products to particulate OM	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A32,A34]	
$H_{Zi,n,j,l,C}$	transfer of microbial C decomposition products to microbial residue	$\text{g C m m}^{-2} \text{ h}^{-1}$	[A38]	
$H_{Zi,n,j,l,N,P}$	transfer of microbial N or P decomposition products to microbial residue	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A39]	
$K_{\lambda N}$	C:N ratio used to calculate internal recycling of C, N	-	[A24a,b]	0.1
$K_{\lambda P}$	C:P ratio used to calculate internal recycling of C, P	-	[A24a,b]	0.01
$K_{is}$	inhibition constant for microbial colonization of substrate	-	[A5]	0.5
$K_{\text{NH}_4}$	M-M constant for $\text{NH}_4^+$ uptake at microbial surfaces	$\text{g N m}^{-3}$	[A26]	0.40
$K_{\text{NO}_3}$	M-M constant for $\text{NO}_3^-$ uptake at microbial surfaces	$\text{g N m}^{-3}$	[A26]	0.35

$K_{\text{PO}_4}$	M-M constant for $\text{H}_2\text{PO}_4^-$ uptake at microbial surfaces	$\text{g P m}^{-3}$	[A26]	0.125	
$K_{iD}$	inhibition constant for $[M_{i,n,a}]$ on $S_{i,C}$ , $Z_{i,C}$	$\text{g C m}^{-3}$	[A4]	25	Grant et al. (1993a,b); Lizama and Suzuki (1990)
$K_{mD}$	Michaelis–Menten constant for $D_{S_{i,C}}$	$\text{g C Mg}^{-1}$	[A4]	75	
$K_{mQ_C}$	Michaelis–Menten constant for $R'_{hi,n}$ on $[Q_{i,C}]$	$\text{g C m}^{-3}$	[A13,A24a]	12	
$K_{O_2}$	Michaelis–Menten constant for reduction of $\text{O}_{2s}$ by microbes, roots and mycorrhizae	$\text{g O}_2 \text{ m}^{-3}$	[A17]	0.064	Griffin (1972); Longmuir (1954)
$k_{ts}$	equilibrium rate constant for sorption	$\text{h}^{-1}$	[A8]	0.01	Grant et al. (1993a,b)
$L_{hj}$	ratio of nonlignin to lignin components in humified hydrolysis products		[A33]	0.10, 0.05, and 0.05 for $j =$ protein, carbohydrate, and cellulose, respectively	Shulten and Schnitzer (1997)
$M$	molecular mass of water	$\text{g mol}^{-1}$	[A15]	18	
$M_{i,d,l,C}$	heterotrophic microbial C used for decomposition	$\text{g C m}^{-2}$	[A1,A3a,A4]		
$M_{i,n,j,l,C}$	microbial C	$\text{g C m}^{-2}$	[A13,A17A23,A24,A25,A26, A30,A36]		
$M_{i,n,j,l,N}$	microbial N	$\text{g N m}^{-2}$	[A18,A23,A24A27,A29]		
$M_{i,n,j,l,P}$	microbial P	$\text{g P m}^{-2}$	[A23,A24,A29,A26, A36]		
$M_{i,n,a,l,C}$	active microbial C from heterotrophic population $n$ associated with $G_{i,l,C}$	$\text{g C m}^{-2}$	[A3,A13,A17, A30]		
$[M_{i,n,a,l,C}]$	concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,l,C} / \theta_l$	$\text{g C m}^{-3}$	[A3, A5]		
$n$	number of microbial microsites	$\text{m}^{-2}$	[A17b]		
$[\text{NH}_4^+]_{i,n,j,l}$	concentration of $\text{NH}_4^+$ at microbial surfaces	$\text{g N m}^{-3}$	[A26]		

$[\text{NH}_4^+_{\text{mn}}]$	concentration of $\text{NH}_4^+$ at microbial surfaces below which $U_{\text{NH}_4} = 0$	$\text{g N m}^{-3}$	[A26]	0.0125	
$[\text{NO}_3^-_{i,n,j,l}]$	concentration of $\text{NH}_4^+$ at microbial surfaces	$\text{g N m}^{-3}$	[A26]		
$[\text{NO}_3^-_{\text{mn}}]$	concentration of $\text{NO}_3^-$ at microbial surfaces below which $U_{\text{NO}_3} = 0$	$\text{g N m}^{-3}$	[A26]	0.03	
$[\text{H}_2\text{PO}_4^-_{i,n,j,l}]$	concentration of $\text{H}_2\text{PO}_4^-$ at microbial surfaces	$\text{g N m}^{-3}$	[A26]		
$[\text{H}_2\text{PO}_4^-_{\text{mn}}]$	concentration of $\text{H}_2\text{PO}_4^-$ at microbial surfaces below which $U_{\text{PO}_4} = 0$	$\text{g N m}^{-3}$	[A26]	0.002	
$[\text{O}_{2\text{mi},n,l}]$	$\text{O}_2$ concentration at heterotrophic microsites	$\text{g O}_2 \text{ m}^{-3}$	[A17]		
$[\text{O}_{2\text{sl}}]$	$\text{O}_2$ concentration in soil solution	$\text{g O}_2 \text{ m}^{-3}$	[A17]		
$Q_{i,l,C}$	$DOC$ from products of $D_{Si,j,l,C}$ [A3] and $D_{Zi,j,l,C}$ [A5]	$\text{g C m}^{-2}$	[A8,A13,A22]		
$[\mathcal{Q}_{i,l,C}]$	solution concentration of $Q_{i,l,C}$	$\text{g C Mg}^{-1}$	[A8,A13,A24a]		
$Q_{i,l,N,P}$	$DON$ and $DOP$ from products of $(D_{Si,j,l,N,P} + D_{Zi,j,l,N,P})$	$\text{g N or P m}^{-2}$	[A9,A22]		
$q_m$	rate constant for reallocating $M_{i,a,l,C}$ to $M_{i,d,l,C}$	$\text{h}^{-1}$	[A3a]	0.5	
$R$	gas constant	$\text{J mol}^{-1} \text{ K}^{-1}$	[A6,A15,C10]	8.3143	
$R_{\phi i,n=f,j,l}$	respiration for non-symbiotic $\text{N}_2$ fixation by heterotrophic diazotrophs ( $n=f$ )	$\text{g C m}^{-2} \text{ h}^{-1}$	[A28]		
$R_{gi,n,l}$	growth respiration of $M_{i,n,a,l}$ on $Q_{i,l,C}$ under nonlimiting $\text{O}_2$ and nutrients	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A20]		
$R_h$	total heterotrophic respiration of all $M_{i,n,a,l}$ under ambient $DOC, \text{O}_2$ , nutrients, $\theta$ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A11]		
$R_{hi,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under ambient $DOC, \text{O}_2$ , nutrients, $\theta$ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A5,A11,A14,A20, A21,A25]		
$R_{hi,n,l}'$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting $\text{O}_2, DOC, \theta$ and $25^\circ\text{C}$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A12,A13]		
$R_h'$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting $DOC, \text{O}_2$ , nutrients, $\theta$ and $25^\circ\text{C}$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A12]	0.125	Shields et al. (1973)

$R'_{h,i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting $O_2$ and ambient DOC, nutrients, $\theta$ and temperature	$g C m^{-2} h^{-1}$	[A13,A14,A16]		
$R_m$	specific maintenance respiration at 25°C	$g C g N^{-1} h^{-1}$	[A18]	0.0115	Barnes et al. (1998)
$R_{mi,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	$g C m^{-2} h^{-1}$	[A18,A20,A21,A25]		
$\sigma$	shape parameter in $f_{\psi g}$	-	[A15]	0.2	Choudhury et al., (2011)
$r_{wl}$	radius of $r_m$ + water film at current water content	m	[A17]		
$r_m$	radius of heterotrophic microsite	m	[A17]	$2.5 \times 10^{-6}$	
$r_{wl}$	thickness of water films	m	[A17]		
$S$	change in entropy	$J mol^{-1} K^{-1}$	[A6,C10]	710	Sharpe and DeMichelle (1977)
$[S_{i,j,l,C}]$	concentration of $S_{i,j,l,C}$ in soil	$g C Mg^{-1}$	[A4a]		
$S_{i,j,l,C}$	mass of colonized litter, POC or humus C	$g C m^{-2}$	[A2a,A5,A7a,A33]		
$S'_{i,j,l,C}$	mass of uncolonized litter, POC or humus C	$g C m^{-2}$	[A5]		
$S_{i,j,l,N,P}$	mass of litter, POC or humus N or P	$g N$ or $P m^{-2}$	[A7a,A33]		
$T_{sl}$	soil temperature	K	[A6,A15,A19]		
$U_{i,n,l,C}$	uptake of $Q_{i,l,C}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	$g C m^{-2} h^{-1}$	[A5,A21,A22,A25]		
$U_{i,n,N,P}$	uptake of $Q_{i,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	$g N$ or $P m^{-2} h^{-1}$	[A22,A29]		
$U_{NH4i,n,j,l}$	$NH_4^+$ uptake by microbes	$g N m^{-2} h^{-1}$	[A26, A27,A29]		
$U'_{NH4}$	maximum $U_{NH4}$ at 25 °C and non-limiting $NH_4^+$	$g N m^{-2} h^{-1}$	[A26]	$5.0 \times 10^{-3}$	
$U_{NO3i,n,j,l}$	$NO_3^-$ uptake by microbes	$g N m^{-2} h^{-1}$	[A26,A27,A29]		

$U'_{\text{NO}_3}$	maximum $U_{\text{NO}_3}$ at 25 °C and non-limiting $\text{NO}_3^-$	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26]	$5.0 \times 10^{-3}$
$U_{\text{O}_2i,n}$	$\text{O}_2$ uptake by $M_{i,n,a,l}$ under ambient $\text{O}_2$	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A17]	
$U'_{\text{O}_2i,n}$	$\text{O}_2$ uptake by $M_{i,n,a,l}$ under nonlimiting $\text{O}_2$	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A16,A17]	
$U_{\text{PO}_4i,n,j,l}$	$\text{H}_2\text{PO}_4^-$ uptake by microbes	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26,A27,A29]	
$U'_{\text{PO}_4}$	maximum $U_{\text{PO}_4}$ at 25 °C and non-limiting $\text{H}_2\text{PO}_4^-$	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26]	$5.0 \times 10^{-3}$
$V_{i,l,C}$	adsorbed C hydrolysis products	$\text{g C Mg}^{-1}$	[A8,A10]	
$V_{i,l,N,P}$	adsorbed N or P hydrolysis products	$\text{g P Mg}^{-1}$	[A10]	
$X_{\text{C}mn}$	minimum C internal recycling fraction	-	[A23a]	0.167
$X_{\text{C}mx}$	maximum C internal recycling fraction	-	[A23a]	0.833
$X_{\text{N,P}}$	maximum N,P internal recycling fraction	-	[A23b]	0.80
$Y_g$	growth yield of aerobic heterotrophs		[A21]	
$y$	selected to give a $Q_{10}$ for $f_{\text{tm}}$ of 2.25		[A19]	0.081
$\psi_s$	soil or residue water potential	$\text{MPa}$	[A15]	
$Y_{i,l,C}$	sorption of C hydrolysis products	$\text{g C m}^{-2} \text{ h}^{-1}$	[A8,A9,A10]	
$Y_{i,l,N,P}$	sorption of N or P hydrolysis products	$\text{g P m}^{-2} \text{ h}^{-1}$	[A9,A10]	
$[Z_{i,j,l,C}]$	concentration of $Z_{i,j,l,C}$ in soil	$\text{g C Mg}^{-1}$	[A4b]	
$Z_{i,j,l,C}$	mass of microbial residue C in soil	$\text{g C m}^{-2}$	[A2b,A7b]	

$Z_{i,j,l,N,P}$ 

mass of microbial residue N or P in soil

 $\text{g P m}^{-2}$ 

[A7b]

## **S2: Soil-Plant Water Relations**

### *Canopy Transpiration*

Canopy energy exchange in *ecosys* is calculated from an hourly two-stage convergence solution for the transfer of water and heat through a multi-layered multi-population soil-root-canopy system. The first stage of this solution requires convergence to a value of canopy temperature  $T_c$  for each plant population at which the first-order closure of the canopy energy balance (net radiation  $R_n$ , latent heat flux  $LE$  [B1a,b,c], sensible heat flux  $H$  [B1d], and change in heat storage  $G$ ) is achieved. These fluxes are controlled by aerodynamic ( $r_a$ ) [B3] and canopy stomatal ( $r_c$ ) [B2] resistances. Two controlling mechanisms are postulated for  $r_c$  which are solved in two successive steps:

- (1) At the leaf level, leaf resistance  $r_l$  [C4] controls gaseous  $\text{CO}_2$  diffusion through each leaf surface when calculating  $\text{CO}_2$  fixation [C1] from concurrent solutions for diffusion  $V_g$  [C2] and carboxylation  $V_c$  [C3]. The value of  $r_l$  is calculated from a minimum leaf resistance  $r_{l\min}$  [C5] for each leaf surface that allows a set ratio for intercellular to canopy  $\text{CO}_2$  concentration  $C_i':C_b$  to be maintained at  $V_c$  under ambient irradiance, air temperature  $T_a$ ,  $C_a$  and zero canopy water potential ( $\psi_c$ ) ( $V_c'$ ). This ratio will be allowed to vary diurnally as described in *Gross Primary Productivity* below when  $\psi_c$  is solved in the second stage of the convergence solution, described under *Water Relations* below. Values of  $r_{l\min}$  are aggregated by leaf surface area to a canopy value  $r_{c\min}$  for use in the energy balance convergence scheme [B2a].
- (2) At the canopy level,  $r_c$  rises from  $r_{c\min}$  at zero  $\psi_c$  from step (1) above through an exponential function of canopy turgor potential  $\psi_t$  [B2b] calculated from  $\psi_c$  and osmotic water potential  $\psi_\pi$  [B4] during convergence for transpiration vs. water uptake.

### *Root and Mycorrhizal Water Uptake*

Root and mycorrhizal water uptake  $U$  [B5] is calculated from the difference between canopy water potential  $\psi_c$  and soil water potential  $\psi_s$  across soil and root hydraulic resistances  $\Omega_s$  [B9] and  $\Omega_r$  [B10 – B12] in each rooted soil layer [B6]. Root resistances are calculated from root radial [B10] and from primary [B11] secondary [B12] axial resistivities using root lengths and surface areas from a root system submodel [B13] driven by exchange of nonstructural C, N and P along concentration gradients generated by uptake vs. consumption of C, N and P in shoots and roots (Grant, 1998).

### *Canopy Water Potential*

After convergence for  $T_c$  is achieved, the difference between canopy transpiration  $E_c$  from the energy balance [B1] and total root water uptake  $U_c$  [B5] from all rooted layers in the soil is tested against the difference between canopy water content from the previous hour and that from the current hour [B14]. This difference is minimized in each iteration by adjusting  $\psi_c$  which in turn determines each of the three terms in [B14]. Because  $r_c$  and  $T_c$  both drive  $E_c$ , the canopy energy balance described under *Canopy Transpiration* above is recalculated for each adjusted value of  $\psi_c$  during convergence.

**Table S2: Soil-Plant Water Relations**

<i>Canopy Transpiration</i>		
$Rn_{ci} + LE_{ci} + H_{ci} + G_{ci} = 0$	canopy energy balance	[B1a]
$LE_{ci} = L (e_a - e_{ci(T_{ci}, \psi_{ci})}) / r_{ai}$	$LE$ from canopy evaporation	[B1b]
$LE_{ci} = L (e_a - e_{ci(T_{ci}, \psi_{ci})}) / (r_{ai} + r_{ci}) - LE_{ci}$ from [B1b]	$LE$ from canopy transpiration	[B1c]
$H_{ci} = \rho C_p (T_a - T_{ci}) / r_{ai}$	$H$ from canopy energy balance	[B1d]
$r_{cmini} = 0.64 (C_b - C_i' i) / V_c' i$	$r_c$ driven by rates of carboxylation vs. diffusion	[B2a]
$r_{ci} = r_{cmini} + (r_{cmaxi} - r_{cmini}) e^{(-\beta \psi_{ti})}$	$r_c$ constrained by water status	[B2b]
$r_{ai} = \{(\ln((z_u - z_{di}) / z_{ri})^2 / (K^2 u_a))\} / (1 - 10 Ri)$	$r_a$ driven by windspeed, surface roughness	[B3a]
$Ri = \{g (z_u - z_{ri}) / (u_a^2 T_a)\} (T_a - T_c)$	$r_a$ adjusted for stability vs. buoyancy	[B3b]
$\psi_{ti} = \psi_{ci} - \psi_{pi}$		[B4]
<i>Root and Mycorrhizal Water Uptake</i>		
$U_{wi} = \sum_l \sum_r U_{wi,r,l}$		[B5]
$U_{wi,r,l} = (\psi_c' i - \psi_s' l) / (\Omega_{si,r,l} + \Omega_{ti,r,l} + \sum_x \Omega_{ai,r,l,x})$	$U_w$ along hydraulic gradient	[B6]
$\psi_c' i = \psi_{ci} + 0.01 z_{bi}$		[B7]
$\psi_s' l = \psi_{sl} - 0.01 z_l$		[B8]
$\Omega_{si,r,l} = \ln\{(d_{i,r,l} / r_{i,r,l}) / (2\pi L_{i,r,l} \kappa_{ti,r,l})\} \theta_{wl} / \theta_{pl}$		[B9]

$$\Omega_{ri,r,l} = \Omega_{ri,r} / L_{i,r,l}$$

[B10]

$$\Omega_{ai,r,l,x=1} = \Omega_{ai,r} z_l / \{n_{i,r,l,1} (r_{i,r,l,1} / r'_{i,r})^4\} + \gamma \Omega_{ai,r} z_{bi} / \{n_{i,r,l,1} (r_{bi} / r'_{bi})^4\} \Sigma_{i,r,l} (M_{i,r,l}) / M_{i,r,l}$$

[B11]

$$\Omega_{ai,r,l,x=2} = \Omega_{ai,r} (L_{i,r,l,2} / n_{i,r,l,2}) / \{n_{i,r,l,2} (r_{i,r,l,2} / r'_{i,r})^4\}$$

[B12]

$$\delta L_{i,r,l,1} / \delta t = \delta M_{i,r,l,1} / \delta t v_r / \{\rho_r (1 - \theta_{P_{i,r}}) (\pi r_{i,r,l,1}^2)\}$$

[B13]

### Canopy Water Potential

$$(e_a - e_{i(T_{ci})}) / (r_{ai} + r_{ci}) [B1] = \Sigma_l \Sigma_r (\psi_c'_{i,l} - \psi_s'_{i,l}) / (\Omega_{si,r,l} + \Omega_{ri,r,l} + \Sigma_x \Omega_{ai,r,l,x}) + X_{ci} \delta \psi_{ci} / \delta t$$

$\psi_c$  solved when transpiration from [B1-B4] (LHS) equals uptake from [B5-B13] + change in storage (RHS)

[B14]

## Definition of Variables in Table S2

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	plant species or functional type: coniferous, deciduous, annual, perennial, C <sub>3</sub> , C <sub>4</sub> , monocot, dicot etc.				
<i>j</i>	branch or tiller				
<i>k</i>	node				
<i>l</i>	soil or canopy layer				
<i>m</i>	leaf azimuth				
<i>n</i>	leaf inclination				
<i>o</i>	leaf exposure (sunlit <i>vs.</i> shaded)				

*r* root or mycorrhizae

*variables*

$\beta$	stomatal resistance shape parameter	MPa <sup>-1</sup>	[B2b,C4,C9]	-5.0	Grant and Flanagan (2007)
$C_b$	[CO <sub>2</sub> ] in canopy air	μmol mol <sup>-1</sup>	[B2,C2,C5]		
$C_i'$	[CO <sub>2</sub> ] in canopy leaves at $\psi_{ci} = 0$ MPa	μmol mol <sup>-1</sup>	[B2]	0.70 $C_b$	Larcher (2001)
$d_{i,r,l}$	half distance between adjacent roots	m	[B9]		
$E_{ci}$	canopy transpiration	m <sup>3</sup> m <sup>-2</sup> h <sup>-1</sup>	[B1,B14]		
$e_a$	atmospheric vapor density at $T_a$ and ambient humidity	g m <sup>-3</sup>	[B1]		
$e_{ci(T_{ci},\psi_{ci})}$	canopy vapor density at $T_{ci}$ and $\psi_{ci}$	g m <sup>-3</sup>	[B1]		
$G_{ci}$	canopy storage heat flux	W m <sup>-2</sup>	[B1]		
$H_{ci}$	canopy sensible heat flux	W m <sup>-2</sup>	[B1]		
$K$	von Karman's constant		[B3a]	0.41	
$\kappa_{ri,r,l}$	hydraulic conductivity between soil and root surface	m <sup>2</sup> MPa <sup>-1</sup> h <sup>-1</sup>	[B9]		
$\gamma$	scaling factor for bole axial resistance from primary root axial resistance	-	[B11]	1.6 x 10 <sup>4</sup>	Grant et al. (2007)
$L$	latent heat of evaporation	J g <sup>-1</sup>	[B1]	2460	
$LE_{ci}$	latent heat flux between canopy and atmosphere	W m <sup>-2</sup>	[B1]		
$L_{i,r,l}$	length of roots or mycorrhizae	m m <sup>-2</sup>	[B9,B10,B12,B13]		
$M_{i,r,l}$	mass of roots or mycorrhizae	g m <sup>-2</sup>	[B11,B13]		
$n_{i,r,l,x}$	number of primary ( $x = 1$ ) or secondary ( $x = 2$ ) axes	m <sup>-2</sup>	[B11,B12]		

$\Omega_{ai,r}$	axial resistivity to water transport along root or mycorrhizal axes	MPa h m <sup>-4</sup>	[B11,B12]	4.0 x 10 <sup>9</sup> deciduous 1.0 x 10 <sup>10</sup> coniferous	Larcher (2001)
$\Omega_{ai,r,l,x}$	axial resistance to water transport along axes of primary ( $x = 1$ ) or secondary ( $x = 2$ ) roots or mycorrhizae	MPa h m <sup>-1</sup>	[B6,B11,B12]		
$\Omega_{ri,r}$	radial resistivity to water transport from surface to axis of roots or mycorrhizae	MPa h m <sup>-2</sup>	[B10]	1.0 x 10 <sup>4</sup>	Doussan et al. (1998)
$\Omega_{ri,r,l}$	radial resistance to water transport from surface to axis of roots or mycorrhizae	MPa h m <sup>-1</sup>	[B6,B10]		
$\Omega_{si,r,l}$	radial resistance to water transport from soil to surface of roots or mycorrhizae	MPa h m <sup>-1</sup>	[B6,B9]		
$\theta_{wl}$	soil water content	m <sup>3</sup> m <sup>-3</sup>	[B9]		
$\theta_{pl}$	soil porosity	m <sup>3</sup> m <sup>-3</sup>	[B9]		
$\theta_{P_{i,r}}$	root porosity	m <sup>3</sup> m <sup>-3</sup>	[B13]		
$Ri$	Richardson number		[B3a,B3b]		van Bavel and Hillel (1976)
$Rn_{ci}$	canopy net radiation	W m <sup>-2</sup>	[B1]		
$r_{ai}$	aerodynamic resistance to vapor flux from canopy	s m <sup>-1</sup>	[B1,B3a]		
$r_{bi}$	radius of bole at ambient $\psi_{ci}$	m	[B11]		
$r_{b'i}$	radius of bole at $\psi_{ci} = 0$ MPa	m	[B11]		
$r_{ci}$	canopy stomatal resistance to vapor flux	s m <sup>-1</sup>	[B1,B2b]		
$r_{cmaxi}$	canopy cuticular resistance to vapor flux	s m <sup>-1</sup>	[B2b]	5.0 x 10 <sup>3</sup>	Larcher (2001)
$r_{cmini}$	minimum $r_{ci}$ at $\psi_{ci} = 0$ MPa	s m <sup>-1</sup>	[B2,B2b]		
$r_{i,r,l,x}$	radius of primary ( $x=1$ ) or secondary ( $x=2$ ) roots or mycorrhizae at ambient $\psi_{ri,l,z}$	m	[B9,B11,B12,B13]		

$r'_{i,r}$	radius of secondary roots or mycorrhizae at $\psi_{r_i,l,z} = 0$ MPa	m	[B11,B12]	2.0 x 10 <sup>-4</sup> tree 1.0 x 10 <sup>-4</sup> bush 0.05 x 10 <sup>-4</sup> mycorrhizae	
$\rho_r$	root specific density	g C g FW <sup>-1</sup>	[B13]	0.05	Grant (1998)
$T_a$	air temperature	K	[B3b]		
$T_c$	canopy temperature	K	[B3b]		
$U_{wi}$	total water uptake from all rooted soil layers	m <sup>3</sup> m <sup>-2</sup> h <sup>-1</sup>	[B5,B14]		
$U_{w,i,r,l}$	water uptake by root and mycorrhizal surfaces in each soil layer	m <sup>3</sup> m <sup>-2</sup> h <sup>-1</sup>	[B5,B6]		
$u_a$	wind speed measured at $z_u$	m s <sup>-1</sup>	[B3a,B3b]		
$V_{c_i}'$	potential canopy CO <sub>2</sub> fixation rate at $\psi_{c_i} = 0$ MPa	µmol m <sup>-2</sup> s <sup>-1</sup>	[B2]		
$v_r$	root specific volume	m <sup>3</sup> g FW <sup>-1</sup>	[B13]	10 <sup>-6</sup>	Grant (1998)
$X_{ci}$	canopy capacitance	m <sup>3</sup> m <sup>-2</sup> MPa <sup>-1</sup>	[B14]		
$\psi_{ci}$	canopy water potential	MPa	[B4,B7,B14]		
$\psi_{c_i}'$	$\psi_{ci}$ + canopy gravitational potential	MPa	[B6,B7]		
$\psi_{ri}$	canopy osmotic potential	MPa	[B4]		
$\psi_{sl}$	soil water potential	MPa	[B8]		
$\psi_s'$	$\psi_{sl}$ + soil gravitational potential	MPa	[B6,B8]		
$\psi_{ti}$	canopy turgor potential	MPa	[B2b,B4]	1.25 at $\psi_c = 0$	
$z_{bi}$	length of bole from soil surface to top of canopy	m	[B7,B11]		
$z_{di}$	canopy zero-plane displacement height	m	[B3a]		Perrier (1982)

$z_l$	depth of soil layer below surface	m	[B8,B11]	
$z_r$	canopy surface roughness	m	[B3a,B3b]	Perrier (1982)
$z_u$	height of wind speed measurement	m	[B3a,B3b]	

### **S3: Gross Primary Productivity, Autotrophic Respiration, Growth and Litterfall**

#### *C<sub>3</sub> Gross Primary Productivity*

After successful convergence for  $T_c$  and  $\psi_c$  (described in *Plant Water Relations* above),  $V_c$  is recalculated from that under zero  $\psi_c$  ( $V_c'$ ) to that under ambient  $\psi_c$ . This recalculation is driven by stomatal effects on  $V_g$  [C2] from the increase in  $r_{lmin}$  at zero  $\psi_c$  [C5] to  $r_c$  at ambient  $\psi_c$  [C4], and by non-stomatal effects  $f_\psi$  [C9] on CO<sub>2</sub>- and light-limited carboxylation  $V_b$  [C6] and  $V_j$  [C7] (Grant and Flanagan, 2007). The recalculation of  $V_c$  is accomplished through a convergence solution for  $C_i$  and its aqueous counterpart  $C_c$  at which  $V_g$  [C2] equals  $V_c$  [C3] (Grant and Flanagan, 2007). The CO<sub>2</sub> fixation rate of each leaf surface at convergence is added to arrive at a value for gross primary productivity (GPP) by each plant population in the model [C1]. The CO<sub>2</sub> fixation product is stored in nonstructural C pools  $\sigma_c$  in each branch.

GPP is strongly controlled by nutrient uptake  $U_{NH_4}$ ,  $U_{NO_3}$  and  $U_{PO_4}$  [C23], products of which are added to nonstructural N ( $\sigma_N$ ) and P ( $\sigma_P$ ) in root and mycorrhizal layers where they are coupled with  $\sigma_c$  to drive growth of branches, roots and mycorrhizae as described in *Growth and Senescence* below. Low  $\sigma_N:\sigma_c$  or  $\sigma_P:\sigma_c$  in branches indicate excess CO<sub>2</sub> fixation with respect to N or P uptake for phytomass growth. Such ratios in the model have two effects on GPP:

- (1) They reduce activities of rubisco [C6a] and chlorophyll [C7a] through product inhibition [C11], thereby simulating the suppression of CO<sub>2</sub> fixation by leaf  $\sigma_c$  accumulation widely reported in the literature.
- (2) They reduce the structural N:C and P:C ratios at which leaves are formed because  $\sigma_c$ ,  $\sigma_N$  and  $\sigma_P$  are the substrates for leaf growth. Lower structural ratios cause a proportional reduction in areal concentrations of rubisco [C6b] and chlorophyll [C7b], reducing leaf CO<sub>2</sub> fixation.

#### *Autotrophic Respiration*

The temperature-dependent oxidation of these nonstructural pools ( $R_c$ ) [C14], plus the energy costs of nutrient uptake [C23], drive autotrophic respiration ( $R_a$ ) [C13] by all branches, roots and mycorrhizae.  $R_c$  by roots and mycorrhizae is constrained by O<sub>2</sub> uptake  $U_{O_2}$  [C14b] calculated by solving for aqueous O<sub>2</sub> concentrations at root and mycorrhizal surfaces [O<sub>2r</sub>] at which convection + radial diffusion through the soil aqueous phase plus radial diffusion through the root aqueous phase [C14d] equals active uptake driven by O<sub>2</sub> demand from  $R_c$  [C14c] (Grant, 2004). These diffusive fluxes are in turn coupled to volatilization – dissolution between aqueous and gaseous phases in soil and root [D14]. The diffusion processes are driven by aqueous O<sub>2</sub> concentrations sustained by

transport and dissolution of gaseous  $O_2$  through soil and roots (Grant 2004), and are governed by lengths and surface areas of roots and mycorrhizae (Grant, 1998). Thus  $R_c$  is coupled to  $O_2$  reduction by all root and mycorrhizal populations according to  $O_2$  availability.  $R_c$  is first used to meet maintenance respiration requirements ( $R_m$ ), calculated independently of  $R_c$  from the N content in each organ, and a function of  $T_c$  or  $T_s$  [C16]. Any excess of  $R_c$  over  $R_m$  is expended as growth respiration  $R_g$ , constrained by branch, root or mycorrhizal  $\psi_t$  [C17]. When  $R_m$  exceeds  $R_c$ , the shortfall is met by the respiration of remobilizable C ( $R_s$ ) in leaves and twigs or roots and mycorrhizae [C15].

#### *Growth and Litterfall*

$R_g$  drives the conversion of branch  $\sigma_C$  into foliage, twigs, branches, boles and reproductive material according to organ growth yields  $Y_g$  and phenology-dependent partitioning coefficients [C20], and the conversion of root and mycorrhizal  $\sigma_C$  into primary and secondary axes according to root and mycorrhizal growth yields. Growth also requires organ-specific ratios of nonstructural N ( $\sigma_N$ ) and P ( $\sigma_P$ ) from  $U_{NH_4}$ ,  $U_{NO_3}$  and  $U_{PO_4}$  [C23] which are coupled with  $\sigma_C$  to drive growth of branches, roots and mycorrhizae.

The translocation of  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  among branches and root and mycorrhizal layers is driven by concentration gradients generated by production of  $\sigma_C$  from branch GPP and of  $\sigma_N$  and  $\sigma_P$  from root and mycorrhizal uptake vs. consumption of  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  from  $R_c$ ,  $R_g$  and phytomass growth (Grant 1998). Low  $\sigma_N:\sigma_C$  or  $\sigma_P:\sigma_C$  in mycorrhizae and roots indicates inadequate N or P uptake with respect to  $CO_2$  fixation. These ratios affect translocation of  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  by lowering mycorrhizal – root – branch concentration gradients of  $\sigma_N$  and  $\sigma_P$  while raising branch – root – mycorrhizal concentration gradients of  $\sigma_C$ . These changes slow transfer of  $\sigma_N$  and  $\sigma_P$  from root to branch and hasten transfer of  $\sigma_C$  from branch to root, increasing root and mycorrhizal growth at the expense of branch growth, and thereby raising N and P uptake [C23] with respect to  $CO_2$  fixation. Conversely, high  $\sigma_N:\sigma_C$  or  $\sigma_P:\sigma_C$  in roots and mycorrhizae indicate excess N or P uptake with respect to  $CO_2$  fixation. Such ratios reduce specific activities of root and mycorrhizal surfaces for N or P uptake through a product inhibition function as has been observed experimentally. These changes hasten transfer of  $\sigma_N$  and  $\sigma_P$  from root to branch and slow transfer of  $\sigma_C$  from branch to root, increasing branch growth at the expense of root and mycorrhizal growth, and thereby slowing N and P uptake. Thus the modelled plant translocates  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  among branches, roots and mycorrhizae to maintain a functional equilibrium between acquisition and use of C, N and P by different parts of the plant.

$R_g$  is limited by  $\psi_t$  [C17], and because branch  $\psi_t$  declines relatively more with soil drying than does root  $\psi_t$ , branch  $R_g$  also declines relatively more with soil drying than does root  $R_g$ , slowing oxidation of  $\sigma_C$  in branches and allowing more translocation of  $\sigma_C$  from branches to roots. This change in allocation of  $\sigma_C$  enables more root growth to reduce  $\Omega_s$ ,  $\Omega_r$  and  $\Omega_a$ , and hence increase  $U$  [B6],

thereby offsetting the effects of soil drying on  $\psi_t$ . Thus the modelled plant translocates  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  among branches, roots and mycorrhizae to maintain a functional equilibrium between acquisition and use of water.

$R_s$  [C15] drives the loss of non-remobilizable C, N and P (mostly structural) as litterfall from leaves and twigs or roots and mycorrhizae [C18a,b,c], and the recycling of remobilizable C, N and P (mostly nonstructural protein) into nonstructural pools  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$ , and depending on ratios of  $\sigma_N:\sigma_C$  or  $\sigma_P:\sigma_C$  [C19a,b,c]. Environmental constraints such as water, heat, nutrient or  $O_2$  stress that reduce  $\sigma_C$  and hence  $R_c$  [C14] with respect to  $R_m$  [C16] increase  $R_s$  [C15] and thereby hasten litterfall [C18]. In addition, concentrations of  $\sigma_C$ ,  $\sigma_N$  and  $\sigma_P$  in roots and mycorrhizae drive exudation of nonstructural C, N and P to DOC, DON and DOP in soil [C19d-h].

$R_a$  of each branch or root and mycorrhizal layer is the total of  $R_c$  and  $R_s$ , and net primary productivity (NPP) is the difference between canopy GPP [C1] and total  $R_a$  of all branches and root and mycorrhizal layers [C13]. Phytomass net growth is the difference between gains driven by  $R_g$  and  $Y_g$ , and losses driven by  $R_s$  and litterfall [C20]. These gains are allocated to leaves, twigs, wood and reproductive material at successive branch nodes, and to roots and mycorrhizae at successive primary and secondary axes, driving leaf expansion [C21a] and root extension [C21b]. Losses from remobilization and litterfall in shoots start at the lowest node of each branch at which leaves or twigs are present, and proceed upwards when leaves or twigs are lost. Losses in roots and mycorrhizae start with secondary axes and proceeds to primary axes when secondary axes are lost.

#### *Root and Mycorrhizal Nutrient Uptake*

Root and mycorrhizal uptake of N and P  $U_{NH_4}$ ,  $U_{NO_3}$  and  $U_{PO_4}$  is calculated by solving for solution  $[NH_4^+]$ ,  $[NO_3^-]$  and  $[H_2PO_4^-]$  at root and mycorrhizal surfaces at which radial transport by mass flow and diffusion from the soil solution to these surfaces [C23a,c,e] equals active uptake by the surfaces [C23b,d,f]. Path lengths and surface areas for  $U_{NH_4}$ ,  $U_{NO_3}$  and  $U_{PO_4}$  are calculated from a root and mycorrhizal growth submodel driven by exchange of nonstructural C, N and P along concentration gradients generated by uptake vs. consumption of C, N and P in shoots and roots (Grant, 1998). A product inhibition function is included to avoid uptake in excess of nutrient requirements [C23g].

#### *C<sub>4</sub> Gross Primary Productivity*

##### *C<sub>4</sub> Mesophyll*

In C<sub>4</sub> plants, the mesophyll carboxylation rate is the lesser of CO<sub>2</sub>- and light-limited reaction rates [C26] (Berry and Farquhar, 1978). The CO<sub>2</sub>-limited rate is a Michaelis-Menten function of PEP carboxylase (PEPc) activity and aqueous CO<sub>2</sub> concentration in the

mesophyll [C29] parameterized from Berry and Farquhar (1978) and from Edwards and Walker (1983). The light-limited rate [C30] is a hyperbolic function of absorbed irradiance and mesophyll chlorophyll activity [C31] with a quantum requirement based on 2 ATP from Berry and Farquhar (1978). PEPC [C32] and chlorophyll [C33] activities are calculated from specific activities multiplied by set fractions of leaf surface N density, and from functions of C<sub>4</sub> product inhibition (Jiao and Chollet, 1988; Lawlor, 1993) [C34],  $\psi_c$  ([C35] as described in Grant and Flanagan, 2007) and  $T_c$  [C10]. Leaf surface N density is controlled by leaf structural N:C and P:C ratios calculated during leaf growth from leaf non-structural N:C and P:C ratios arising from root N and P uptake (Grant, 1998) vs. CO<sub>2</sub> fixation.

#### *C<sub>4</sub> Mesophyll-Bundle Sheath Exchange*

Differences in the mesophyll and bundle sheath concentrations of the C<sub>4</sub> carboxylation product drive mesophyll-bundle sheath transfer (Leegood, 2000) [C37]. The bundle sheath concentration of the C<sub>4</sub> product drives a product-inhibited decarboxylation reaction (Laisk and Edwards, 2000) [C38], the CO<sub>2</sub> product of which generates a concentration gradient that drives leakage of CO<sub>2</sub> from the bundle sheath to the mesophyll [C39]. CO<sub>2</sub> in the bundle sheath is maintained in 1:50 equilibrium with HCO<sub>3</sub><sup>-</sup> (Laisk and Edwards, 2000). At this stage of model development, the return of a C<sub>3</sub> decarboxylation product from the bundle sheath to the mesophyll is not simulated. Parameters used in Eqs. [C37 – C39] allowed mesophyll and bundle sheath concentrations of C<sub>4</sub> carboxylation products from [C40 – C41] to be maintained at values consistent with those in Leegood (2000), bundle sheath concentrations of CO<sub>2</sub> (from Eq. [C42]) to be maintained at values similar to those reported by Furbank and Hatch (1987), and bundle sheath CO<sub>2</sub> leakiness [C39]), expressed as a fraction of PEP carboxylation, to be maintained at values similar to those in Williams et al. (2001), in sorghum as described in Grant et al. (2004).

#### *C<sub>4</sub> Bundle Sheath*

A C<sub>3</sub> model in which carboxylation is the lesser of CO<sub>2</sub>- and light-limited reaction rates (Farquhar et al., 1980) has been parameterized for the bundle sheath of C<sub>4</sub> plants [C43] from Seeman et al. (1984). The CO<sub>2</sub>-limited rate [C44] is a Michaelis-Menten function of RuBP carboxylase (RuBPc) activity and bundle sheath CO<sub>2</sub> concentration [C42]. The light-limited rate [C45a] is a hyperbolic function of absorbed irradiance and activity of chlorophyll associated with the bundle sheath with a quantum yield based on 3 ATP [C46]. The provision of reductant from the mesophyll to the bundle sheath in NADP-ME species is not explicitly simulated. RuBPc [C47] and chlorophyll [C48] activities are the products of specific activities and concentrations multiplied by set fractions of leaf surface N density, and from functions of C<sub>3</sub> product inhibition (Bowes, 1991; Stitt, 1991) [C49],  $\psi_c$  (Eq. A12 from Grant and Flanagan, 2007) and  $T_c$  [C10].

Rates of C<sub>3</sub> product removal are controlled by phytomass biosynthesis rates driven by concentrations of nonstructural products from leaf CO<sub>2</sub> fixation and from root N and P uptake. If biosynthesis rates are limited by nutrient uptake, consequent depletion of nonstructural N or P and accumulation of nonstructural C will constrain specific activities of RuBP and chlorophyll [C47 – C49], and thereby slow C<sub>3</sub> carboxylation [C43], raise bundle sheath CO<sub>2</sub> concentration [C42], accelerate CO<sub>2</sub> leakage [C39], slow C<sub>4</sub> decarboxylation [C38], raise C<sub>4</sub> product concentration in the bundle sheath [C41], slow C<sub>4</sub> product transfer from the mesophyll [C37], raise C<sub>4</sub> product concentration in the mesophyll [C40], and slow mesophyll CO<sub>2</sub> fixation [C32 – C35]. This reaction sequence simulates the progressive inhibition of C<sub>3</sub> and C<sub>4</sub> carboxylation hypothesized by Sawada et al. (2002) following partial removal of C sinks in C<sub>4</sub> plants.

#### *Shoot – Root - Mycorrhizal C, N, P Transfer*

Shoot – root C transfers  $Z_{sC}$  are calculated such that concentrations of  $\sigma_C$  with respect to structural phytomass in each branch and root layer approach equilibrium according to conductances  $g_{sC}$  calculated from shoot – root distances and axis numbers in each root layer [C50] (Grant, 1998). Because  $\sigma_C$  is generated by CO<sub>2</sub> fixation in branches [C1],  $g_{sC}$  cause shoot-to-root gradients of  $\sigma_C$  that drive  $Z_{sC}$ . Shoot – root N and P transfers  $Z_{sN,P}$  are calculated such that concentrations of  $\sigma_{N,P}$  with respect to  $\sigma_C$  in each branch and root layer approach equilibrium according to rate constants  $g_{sN,P}$  [C51]. Because  $\sigma_{N,P}$  are generated by uptake in roots [C23],  $g_{sN,P}$  cause root-to-shoot gradients of  $\sigma_{N,P}$  that drive  $Z_{sN,P}$ .

Similarly, root - mycorrhizal C transfers  $Z_{rC}$  are calculated such that concentrations of  $\sigma_C$  with respect to structural phytomass in each root and mycorrhizal layer approach equilibrium according to rate constants  $g_{rC}$  [C52] (Grant, 1998). Because  $\sigma_C$  is maintained by  $Z_{sC}$  [C50],  $g_{rC}$  cause root-to-mycorrhizal gradients of  $\sigma_C$  that drive  $Z_{rC}$ . Root - mycorrhizal N and P transfers  $Z_{rN,P}$  are calculated such that concentrations of  $\sigma_{N,P}$  with respect to  $\sigma_C$  in each root and mycorrhizal layer approach equilibrium according to rate constants  $g_{rN,P}$  [C53]. Because mycorrhizal  $\sigma_{N,P}$  are generated by uptake with greater surface area and length with respect to phytomass [C23],  $g_{rN,P}$  cause mycorrhizal-to-root gradients of  $\sigma_{N,P}$  that drive  $Z_{rN,P}$ .

**Table S3: Gross Primary Productivity, Autotrophic Respiration, Growth and Litterfall**

<i>C<sub>3</sub> Gross Primary Productivity</i>	
$CPP = \sum_{i,j,k,l,m,n,o} (V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}) A_{i,j,k,l,m,n,o} \mathbf{C} \mathbf{F}_i$	solve for $C_{ii,j,k,l,m,n,o}$ at which [C1]
$V_{gi,j,k,l,m,n,o} = (C_b - C_{ii,j,k,l,m,n,o}) / r_{li,j,k,l,m,n,o}$	$V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}$ diffusion [C2]
$V_{ci,j,k,l,m,n,o} = \min\{V_{bi,j,k,l,m,n,o}, V_{ji,j,k,l,m,n,o}\}$	carboxylation [C3]
$r_{li,j,k,l,m,n,o} = r_{lmini,j,k,l,m,n,o} + (r_{lmaxi} - r_{lmini,j,k,l,m,n,o}) e^{(-\beta \psi_i)}$	$r_l$ is leaf-level equivalent of $r_c$ [C4]
$r_{lmini,j,k,l,m,n,o} = (C_b - \mathbf{C}_i' \mathbf{i}) / V_{ci,j,k,l,m,n,o}$	minimum $r_l$ is driven by [C5]
$V_{bi,j,k,l,m,n,o} = V_{bmaxi,j,k} (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (C_{ci,j,k,l,m,n,o} + K_{ci}) f_{\psi i,j,k,l,m,n,o}$	carboxylation [C6a]
$V_{bmaxi,j,k} = \mathbf{V}_b' \mathbf{F}_{rubiscoi} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{tbi} f_{iCi}$	$CO_2$ and water $f_{\psi}$ constraints on $V_b$ [C6a]
$\Gamma_{i,j,k} = 0.5 O_c V_{omaxi,j,k} \mathbf{K}_{ci} / (V_{bmaxi,j,k} \mathbf{K}_{oi})$	temperature $f_{tb}$ and nutrient $f_{iC}$ [C6b]
$V_{omaxi,j,k} = \mathbf{V}_o' \mathbf{F}_{rubiscoi} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{toi}$	constraints on $V_{bmax}$ [C6b]
$K_{ci} = \mathbf{K}_{ci} f_{tkci} (1 + O_c / (\mathbf{K}_{oi} f_{tkoi}))$	$CO_2$ compensation point [C6c]
$V_{ji,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o} Y_{i,j,k,l,m,n,o} f_{\psi i,j,k,l,m,n,o}$	oxygenation [C6d]
$Y_{i,j,k,l,m,n,o} = (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (4.5 C_{ci,j,k,l,m,n,o} + 10.5 \Gamma_{i,j,k})$	$M\text{-}M$ constant for $V_b$ [C6e]
$J_{i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{maxi,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{maxi,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{maxi,j,k})^{0.5}) / (2\alpha)$	water constraints on $V_j$ [C7a]
$J_{maxi,j,k} = \mathbf{V}_j' \mathbf{F}_{chlorophylli} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{tji} f_{iCi}$	carboxylation efficiency of $V_j$ [C7b]
	irradiance constraints on $J$ [C8a]
	temperature and nutrient [C8b]
	constraints on $J_{max}$

$$f_{\psi i,j,k,l,m,n,o} = (r_{\text{lmin}_{i,j,k,l,m,n,o}} / r_{i,j,k,l,m,n,o})^{0.5}$$

$$f_{\text{tbi}} = \exp[\mathbf{B}_v - \mathbf{H}_{\text{av}} / (\mathbf{R}T_{ci})] / \{1 + \exp[(\mathbf{H}_{\text{dl}} - ST_{ci}) / (\mathbf{R}T_{ci})] + \exp[(ST_{ci} - \mathbf{H}_{\text{dh}}) / (\mathbf{R}T_{ci})]\}$$

$$f_{\text{toi}} = \exp[\mathbf{B}_o - \mathbf{H}_{\text{ao}} / (\mathbf{R}T_{ci})] / \{1 + \exp[(\mathbf{H}_{\text{dl}} - ST_{ci}) / (\mathbf{R}T_{ci})] + \exp[(ST_{ci} - \mathbf{H}_{\text{dh}}) / (\mathbf{R}T_{ci})]\}$$

$$f_{\text{tj}} = \exp[\mathbf{B}_j - \mathbf{H}_{\text{aj}} / (\mathbf{R}T_{ci})] / \{1 + \exp[(\mathbf{H}_{\text{dl}} - ST_{ci}) / (\mathbf{R}T_{ci})] + \exp[(ST_{ci} - \mathbf{H}_{\text{dh}}) / (\mathbf{R}T_{ci})]\}$$

$$f_{\text{tkci}} = \exp[\mathbf{B}_{\text{kc}} - \mathbf{H}_{\text{akc}} / (\mathbf{R}T_{ci})]$$

$$f_{\text{tkoi}} = \exp[\mathbf{B}_{\text{ko}} - \mathbf{H}_{\text{ako}} / (\mathbf{R}T_{ci})]$$

$$f_{\text{Ci}} = \min\{\sigma_{\text{Ni},j} / (\sigma_{\text{Ni},j} + \sigma_{\text{Ci},j} / K_{\text{ICN}}), \sigma_{\text{Pi},j} / (\sigma_{\text{Pi},j} + \sigma_{\text{Ci},j} / K_{\text{ICP}})\}$$

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

### Autotrophic Respiration

$$R_a = \sum_i \sum_j (R_{ci,j} + R_{si,j}) + \sum_i \sum_l \sum_z (R_{ci,r,l} + R_{si,r,l}) + E_{N,P} (U_{\text{NH4i},r,l} + U_{\text{NO3i},r,l} + U_{\text{PO4i},r,l})$$

$$R_{ci,j} = R_c' \sigma_{Ci,j} f_{\text{ta}}$$

$$R_{ci,r,l} = R_c' \sigma_{C,i,r,l} f_{\text{ta},i,l} (U_{\text{O2i},r,l} / U'_{\text{O2i},r,l})$$

$$U_{\text{O2i},r,l} = U'_{\text{O2i},r,l} [\text{O}_{2ri},r,l] / ([\text{O}_{2ri},r,l] + K_{\text{O}_2})$$

$$\begin{aligned} &= U_{\text{w}_{i,r,l}} [\text{O}_{2sl}] + 2\pi L_{i,r,l} D_{\text{so2}} ([\text{O}_{2sl}] - [\text{O}_{2ri},r,l]) \ln\{(\text{r}_{sl} + \text{r}_{ri,r,l}) / \text{r}_{ri,r,l}\} \\ &\quad + 2\pi L_{i,r,l} D_{\text{ro2}} ([\text{O}_{2qi},r,l] - [\text{O}_{2ri},r,l]) \ln(\text{r}_{qi,r,l}) / \text{r}_{ri,r,l} \end{aligned}$$

$$U'_{\text{O2i},r,l} = 2.67 R_a'_{i,r,l}$$

non-stomatal effect related to stomatal effect [C9]

Arrhenius functions for carboxylation, oxygenation and electron transport [C10a]

temperature sensitivity of  $K_{ci}, K_{oi}$  [C10b]

[C10c]

[C10d]

[C10e]

control of  $\sigma_N$  and  $\sigma_P$  vs.  $\sigma_C$  in shoots on  $V_b, V_j$  through product inhibition and on leaf protein growth through leaf structural C:N:P ratios [C11]

growth of remobilizable leaf protein C [C12]

total autotrophic respiration [C13]

$O_2$  constraint on root respiration from active uptake coupled with diffusion of  $O_2$  from soil as for heterotrophic respiration in [A17], and from active uptake coupled with diffusion of  $O_2$  from roots [C14a]

[C14b]

[C14c]

[C14d]

[C14e]

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

remobilization in branchs, roots and mycorrhizae when  $R_m > R_c$  [C15]

$$R_{si,r,l} = - \min\{0.0, R_{ci,r,l} - R_{mi,r,l}\}$$

$$R_{mi,j} = \sum_z (N_{i,j,z} \mathbf{R}_m' f_{tmj})$$

maintenance respiration of branchs, roots and mycorrhizae [C16]

$$R_{mi,r,l} = \sum_z (N_{i,r,l,z} \mathbf{R}_m' f_{tmj})$$

$$R_{gi,j} = \max\{0.0, \min\{(R_{ci,j} - R_{mi,j}) \min\{1.0, \max\{0.0, \psi_{ti} - \psi_t'\}\}\}$$

growth respiration of branchs, roots and mycorrhizae when  $R_m < R_c$  [C17]

$$R_{gi,r,l} = \max\{0.0, \min\{(R_{ci,r,l} - R_{mi,r,l}) \min\{1.0, \max\{0.0, \psi_{ti,l} - \psi_t'\}\}\}$$

### *Growth and Litterfall*

$$l_{i,j,z,C} = R_{si,j} M_{L_{N^{i,j}}} / M_{L_{R^{i,j}}} (1.0 - (X_{Cmn} + (X_{Cmx} - X_{Cmn}) f_{\lambda Ci,j}))$$

senescence drives litterfall of non-remobilizable C less C recycling [C18a]

$l_{i,j,z,\text{N}} = l_{i,j,z,\text{C}} \mathbf{N}_{\text{prot}} (1.0 - X_{\text{N}} f_{\lambda,\text{Ni},j})$	[C18b]
$l_{i,j,z,\text{P}} = l_{i,j,z,\text{C}} \mathbf{P}_{\text{prot}} (1.0 - X_{\text{P}} f_{\lambda,\text{Pi},j})$	[C18c]
$f_{\lambda,\text{Ci},j} = \min \{ \sigma_{\text{Ni},j} / (\sigma_{\text{Ni},j} + \sigma_{\text{Ci},j} K_{\lambda,\text{N}}), \sigma_{\text{Pi},j} / (\sigma_{\text{Pi},j} + \sigma_{\text{Ci},j} K_{\lambda,\text{P}}) \}$	[C19a]
$f_{\lambda,\text{Ni},j} = \sigma_{\text{Ci},j} / (\sigma_{\text{Ci},j} + \sigma_{\text{Ni},j} / K_{\lambda,\text{N}})$	[C19b]
$f_{\lambda,\text{Pi},j} = \sigma_{\text{Ci},j} / (\sigma_{\text{Ci},j} + \sigma_{\text{Pi},j} / K_{\lambda,\text{P}})$	[C19c]
$x_{i,r,l,\text{C}} = r_x \sigma_{\text{Ci},r,l}$	[C19d]
$x_{i,r,l,\text{N}} = r_x \sigma_{\text{Ni},r,l} f_{x_{i,r,l},\text{N}}$	[C19e]
$x_{i,r,l,\text{P}} = r_x \sigma_{\text{Pi},r,l} f_{x_{i,r,l},\text{P}}$	[C19f]
$f_{x_{i,r,l},\text{N}} = \sigma_{\text{Ni},j} / (\sigma_{\text{Ni},j} + \sigma_{\text{Ci},j} / K_{x,\text{N}})$	[C19g]
$f_{x_{i,r,l},\text{P}} = \sigma_{\text{Pi},j} / (\sigma_{\text{Pi},j} + \sigma_{\text{Ci},j} / K_{x,\text{P}})$	[C19h]
$\delta M_{\text{B}_{i,j}} / \delta t = \sum_z [R_{\text{g}_{i,j}} (1 - Y_{\text{g}_{i,z}}) / Y_{\text{g}_{i,z}}] - R_{\text{s}_{i,j}} - l_{i,j,\text{C}}$	branch growth driven by $R_g$ [C20a]
$\delta M_{\text{R}_{i,r,l}} / \delta t = [R_{\text{g}_{i,r,l}} (1 - Y_{\text{g}_{i,r}}) / Y_{\text{g}_{i,r}}] - R_{\text{s}_{i,r,l}} - l_{i,r,l,\text{C}}$	root growth driven by $R_g$ [C20b]
$\delta A_{\text{L}_{i,j,k,l}} / \delta t = \chi (M_{\text{L}_{i,j,k,l}} / y_i)^{-0.33} \delta M_{\text{L}_{i,j,k,l}} / \delta t \min \{ 1, \max \{ 0, \psi_{ti} - \psi_t' \} \}$	leaf expansion driven by leaf mass growth [C21a]
$\delta L_{i,r,l,1} / \delta t = (\delta M_{\text{R}_{i,r,l,1}} / \delta t) / y_i v_r / \{ \rho_r (1 - \theta_{\text{P}_{i,r}}) (\pi r_{i,r,l,1}^2) \}$	root extension of primary and secondary axes driven by root mass growth [C21b]
$\delta L_{i,r,l,2} / \delta t = (\delta M_{\text{R}_{i,r,l,2}} / \delta t) v_r / \{ \rho_r (1 - \theta_{\text{P}_{i,r}}) (\pi r_{i,r,l,2}^2) \}$	[C21c]
$f_{\text{ta}_i} = T_{ci} \{ \exp[\mathbf{B}_{\text{v}} - \mathbf{H}_{\text{av}} / (\mathbf{R}T_{ci})] \} / \{ 1 + \exp[(\mathbf{H}_{\text{dl}} - ST_{ci}) / (\mathbf{R}T_{ci})] + \exp[(ST_{ci} - \mathbf{H}_{\text{dh}}) / (\mathbf{R}T_{ci})] \}$	Arrhenius function for $R_a$ [C22a]
$f_{\text{tm}_i} = e^{(0.0811 (T_{ci} - 298.15))}$	temperature function for $R_m$ [C22b]

### Root and Mycorrhizal Nutrient Uptake

$U_{\text{NH4}i,r,l} = \{ U_{\text{wi},r,l} [\text{NH}_4^+]_l + 2\pi L_{i,r,l} D_{\text{eNH4}l} ([\text{NH}_4^+]_l - [\text{NH}_4^+_{i,r,l}]) / \ln(d_{i,r,l} / r_{ri,r,l}) \}$ $= U'_{\text{NH4}} (U_{\text{O2}i,r,l} / U'_{\text{O2}i,r,l}) A_{i,r,l} ([\text{NH}_4^+]_l - [\text{NH}_4^+_{\text{mn}}]) / ([\text{NH}_4^+]_l - [\text{NH}_4^+_{\text{mn}}] + K_{\text{NH4}}) f_{\text{tai},l} f_{\text{iNi},r,l}$	[C23a] [C23b]
$U_{\text{NO3}i,r,l} = \{ U_{\text{wi},r,l} [\text{NO}_3^-]_l + 2\pi L_{i,r,l} D_{\text{eNO3}l} ([\text{NO}_3^-]_l - [\text{NO}_3^-_{i,r,l}]) / \ln(d_{i,r,l} / r_{ri,r,l}) \}$ $= U'_{\text{NO3}} (U_{\text{O2}i,r,l} / U'_{\text{O2}i,r,l}) A_{i,r,l} ([\text{NO}_3^-]_l - [\text{NO}_3^-_{\text{mn}}]) / ([\text{NO}_3^-]_l - [\text{NO}_3^-_{\text{mn}}] + K_{\text{NO3}}) f_{\text{tai},l} f_{\text{iNi},r,l}$	[C23c] [C23d]
$U_{\text{PO4}i,r,l} = \{ U_{\text{wi},r,l} [\text{H}_2\text{PO}_4^-]_l + 2\pi L_{i,r,l} D_{\text{ePO4}l} ([\text{H}_2\text{PO}_4^-]_l - [\text{H}_2\text{PO}_4^-_{i,r,l}]) / \ln(d_{i,r,l} / r_{ri,r,l}) \}$ $= U'_{\text{PO4}} (U_{\text{O2}i,r,l} / U'_{\text{O2}i,r,l}) A_{i,r,l} ([\text{H}_2\text{PO}_4^-]_l - [\text{H}_2\text{PO}_4^-_{\text{mn}}]) / ([\text{H}_2\text{PO}_4^-]_l - [\text{H}_2\text{PO}_4^-_{\text{mn}}] + K_{\text{PO4}}) f_{\text{tai},l} f_{\text{iPi},r,l}$	[C23e] [C23f]
$f_{\text{iNi},r,l} = \sigma_{\text{Ci},r,l} / (\sigma_{\text{Ci},r,l} + \sigma_{\text{Ni},r,l} / K_{\text{iNc}})$	[C23g]
$f_{\text{iPi},r,l} = \sigma_{\text{Ci},r,l} / (\sigma_{\text{Ci},r,l} + \sigma_{\text{Pi},r,l} / K_{\text{iPc}})$	[C23h]

#### *C<sub>4</sub> Gross Primary Productivity*

##### *C<sub>4</sub> Mesophyll*

$GPP = \sum_{i,j,k,l,m,n,o} (V_{\text{g(m4)}i,j,k,l,m,n,o} - V_{\text{c(m4)}i,j,k,l,m,n,o})$	[C24]
$V_{\text{g(m4)}i,j,k,l,m,n,o} = (C_b - C_{\text{i(m4)}i,j,k,l,m,n,o}) / r_{\text{lf},i,j,k,l,m,n,o}$	[C25]
$V_{\text{c(m4)}i,j,k,l,m,n,o} = \min\{V_{\text{b(m4)}i,j,k,l,m,n,o}, V_{\text{j(m4)}i,j,k,l,m,n,o}\}$	[C26]
$r_{\text{lf},i,j,k,l,m,n,o} = r_{\text{lf},\text{mini},i,j,k,l,m,n,o} + (r_{\text{lf},\text{maxi}} - r_{\text{lf},\text{mini},i,j,k,l,m,n,o}) e^{(-\beta \psi_i)}$	[C27]
$r_{\text{lf},\text{mini},i,j,k,l,m,n,o} = (C_b - C_{\text{i(m4)}'i}) / V_{\text{c0(m4)}i,j,k,l,m,n,o}$	[C28]
$V_{\text{b(m4)}i,j,k,l,m,n,o} = V_{\text{bmax(m4)}i,j,k} (C_{\text{c(m4)}i,j,k,l,m,n,o} - \Gamma_{\text{(m4)}i,j,k}) / (C_{\text{c(m4)}i,j,k,l,m,n,o} + K_{\text{c(m4)}i,j,k})$	[C29]
$V_{\text{j(m4)}i,j,k,l,m,n,o} = J_{\text{(m4)}i,j,k,l,m,n,o} Y_{\text{(m4)}i,j,k,l,m,n,o}$	[C30a]
$Y_{\text{(m4)}i,j,k} = (C_{\text{c(m4)}i,j,k,l,m,n,o} - \Gamma_{\text{(m4)}i,j,k}) / (3.0 C_{\text{c(m4)}i,j,k,l,m,n,o} + 10.5 \Gamma_{\text{(m4)}i,j,k})$	[C30b]
$J_{\text{(m4)}i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\text{max(m4)}i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\text{max(m4)}i,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\text{max(m4)}i,j,k})^{0.5}) / (2\alpha)$	[C31]
$V_{\text{bmax(m4)}i,j,k} = V_{\text{bmax(m4)}}' [N_{\text{pep(m4)}i,j,k}]' N_{\text{lf},i,j,k} A_{\text{lf},i,j,k} f_{\text{C(m4)}i,j,k} f_{\psi i} f_{\text{tbi}}$	[C32]

$J_{\max(m4)i,j,k} = J_{\max}' [N_{\text{chl}(m4)i,j,k}]' N_{\text{lf}(i,j,k}} A_{\text{lf}(i,j,k}} f_{C(m4)i,j,k} f_{\psi i} f_{tij}$	chlorophyll activity	[C33]
$f_{C(m4)i,j,k} = 1.0 / (1.0 + [\chi_{C4(m4)i,j,k}] / K_{\chi_{C4(m4)}})$	$C_4$ product inhibition	[C34]
$f_{\psi i,j,k,l,m,n,o} = (r_{\text{lfmin},i,j,k,l,m,n,o} / r_{\text{lf},i,j,k,l,m,n,o})^{0.5}$	non-stomatal water limitation	[C35]

#### $C_4$ Mesophyll-Bundle Sheath Exchange

$V_{\chi_{C4(m4)i,j,k}} = \kappa_{\chi_{C4(m4)}} (\chi_{C4(m4)i,j,k} W_{\text{lf}(b4)i,j,k} - \chi_{C4(b4)i,j,k} W_{\text{lf}(m4)i,j,k}) / (W_{\text{lf}(b4)i,j,k} + W_{\text{lf}(m4)i,j,k})$	mesophyll-bundle sheath transfer	[C37]
$V_{\chi_{C4(b4)i,j,k}} = \kappa_{\chi_{C4(b4)}} \chi_{C4(b4)i,j,k} / (1.0 + C_{c(b4)i,j,k} / K_{\chi_{C4(b4)}})$	bundle sheath decarboxylation	[C38]
$V_{\phi(b4)i,j,k} = \kappa_{C_c(b4)} (C_{c(b4)i,j,k} - C_{c(m4)i,j,k}) (12 \times 10^{-9}) W_{\text{lf}(b4)i,j,k}$	bundle sheath-mesophyll leakage	[C39]
$\delta \chi_{C4(m4)i,j,k} / \delta t = \sum_{l,m,n,o} V_{c(m4)i,j,k,l,m,n,o} - V_{\chi_{C4(m4)i,j,k}}$	mesophyll carboxylation products	[C40]
$\delta \chi_{C4(b4)i,j,k} / \delta t = V_{\chi_{C4(m4)i,j,k}} - V_{\chi_{C4(b4)i,j,k}}$	bundle sheath carboxylation products	[C41]
$\delta C_{c(b4)i,j,k} / \delta t = V_{\chi_{C4(b4)i,j,k}} - V_{\phi(b4)i,j,k} - \sum_{l,m,n,o} V_{c(b4)i,j,k,l,m,n,o}$	bundle sheath $\text{CO}_2$ concentration	[C42]

#### $C_4$ Bundle Sheath

$V_{c(b4)i,j,k,l,m,n,o} = \min\{V_{b(b4)i,j,k}, V_{j(b4)i,j,k,l,m,n,o}\}$	bundle sheath carboxylation	[C43]
$V_{b(b4)i,j,k} = V_{\text{bmax}(b4)i,j,k} (C_{c(b4)i,j,k} - \Gamma_{(b4)i,j,k}) / (C_{c(b4)i,j,k} + K_{c(b4)i,j,k})$	$\text{CO}_2$ -limited carboxylation	[C44]
$V_{j(b4)i,j,k,l,m,n,o} = J_{(b4)i,j,k,l,m,n,o} Y_{(b4)i,j,k}$	light- limited carboxylation	[C45a]
$Y_{(b4)i,j,k} = (C_{c(b4)i,j,k} - \Gamma_{(b4)i,j,k}) / (4.5 C_{c(b4)i,j,k} + 10.5 \Gamma_{(b4)i,j,k})$	carboxylation efficiency of $V_{j(b4)}$	[C45b]
$J_{(b4)i,j,k,l,m,n,o} = (\mathcal{E} I_{i,l,m,n,o} + J_{\max(b4)i,j,k} - ((\mathcal{E} I_{i,l,m,n,o} + J_{\max(b4)i,j,k})^2 - 4\alpha\mathcal{E} I_{i,l,m,n,o} J_{\max(b4)i,j,k})^{0.5}) / (2\alpha)$	irradiance response function	[C46]
$V_{\text{bmax}(b4)i,j,k} = V_{\text{bmax}(b4)}' [N_{\text{rub}(b4)i,j,k}]' N_{\text{lf}(i,j,k}} A_{\text{lf}(i,j,k}} f_{C(c3)i,j,k} f_{\psi i} f_{tvi}$	RuBPc activity	[C47]
$J_{\max(b4)i,j,k} = J_{\max}' [N_{\text{chl}(b4)i,j,k}]' N_{\text{lf}(i,j,k}} A_{\text{lf}(i,j,k}} f_{C(c3)i,j,k} f_{\psi i} f_{tvi}$	chlorophyll activity	[C48]

$$f_{C(c3)i,j,k} = \min\{ [v_{lfi,j}] / ([v_{lfi,j}] + [\chi_{c3(b4)i,j}] / K_{lvi_lf}), [\pi_{lfi,j}] / ([\pi_{lfi,j}] + [\chi_{c3(b4)i,j}] / K_{lpi_lf}) \} \quad C_3 \text{ product inhibition} \quad [C49]$$

### Shoot – Root - Mycorrhizal C, N, P Transfer

$$Z_{sCi,j-i,r,l} = g_{sCi,j-i,r,l} (\sigma_{Ci,j} M_{Ri,r,l} - \sigma_{Ci,r,l} M_{Bi,j}) / (M_{Ri,r,l} + M_{Bi,j}) \quad \text{shoot – root C transfer driven by } \sigma_C \text{ concentration gradients} \quad [C50]$$

$$Z_{sN,Pi,j-i,r,l} = g_{sN,Pi,j-i,r,l} (\sigma_{N,Pi,j} \sigma_{Ci,r,l} - \sigma_{N,Pi,r,l} \sigma_{Ci,j}) / (\sigma_{Ci,r,l} + \sigma_{Ci,j}) \quad \text{shoot – root N,P transfer driven by } \sigma_{N,P} \text{ concentration gradients} \quad [C51]$$

$$Z_{rCi,j-i,r,l} = g_{rCi,j-i,r,l} (\sigma_{Ci,r,l} M_{Mi,r,l} - \sigma_{Ci,m,l} M_{Ri,r,l}) / (M_{Mi,r,l} + M_{Ri,r,l}) \quad \text{root – mycorrhizal C transfer driven by } \sigma_C \text{ conc'n gradients} \quad [C52]$$

$$Z_{rN,Pi,j-i,r,l} = g_{rN,Pi,j-i,r,l} (\sigma_{N,Pi,r,l} \sigma_{Ci,m,l} - \sigma_{N,Pi,m,l} \sigma_{Ci,r,l}) / (\sigma_{Ci,m,l} + \sigma_{Ci,r,l}) \quad \text{root – mycorrhizal N,P transfer driven by } \sigma_{N,P} \text{ conc'n gradients} \quad [C53]$$

### Definition of Variables in Table S3

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	species or functional type: evergreen, coniferous, deciduous, annual, perennial, C <sub>3</sub> , C <sub>4</sub> , monocot, dicot, legume etc.				
<i>j</i>	branch or tiller				
<i>k</i>	node				
<i>l</i>	soil or canopy layer				
<i>m</i>	leaf azimuth				
<i>n</i>	leaf inclination				
<i>o</i>	leaf exposure (sunlit <i>vs.</i> shaded)				
<i>z</i>	organ including leaf, stem, root <i>r</i> , mycorrhizae <i>m</i>				
<i>variables</i>					
<i>A</i>	Leaf (irradiated), root or mycorrhizal surface area	m <sup>2</sup> m <sup>-2</sup>		[C1,C6b,C6d,C8b, C21,C23,C32,C33, C47]	
<i>β</i>	shape parameter for stomatal effects on CO <sub>2</sub> diffusion and non-stomatal effects on carboxylation	MPa <sup>-1</sup>	[C4 C27,C35,]	-5.0	Grant and Flanagan (2007)

$B_j$	parameter such that $f_{iji} = 1.0$ at $T_c = 298.15$ K		[C10c]	17.354
$B_{kc}$	parameter such that $f_{tkci} = 1.0$ at $T_c = 298.15$ K		[C10d]	22.187
$B_{ko}$	parameter such that $f_{tkoi} = 1.0$ at $T_c = 298.15$ K		[C10e]	8.067
$B_o$	parameter such that $f_{toi} = 1.0$ at $T_c = 298.15$ K		[C10b]	24.212
$B_v$	parameter such that $f_{tvi} = 1.0$ at $T_c = 298.15$ K		[C10a, C22]	26.229
$C_b$	[CO <sub>2</sub> ] in canopy air	μmol mol <sup>-1</sup>	[C2,C5 C25,C28]	
$C_c$	[CO <sub>2</sub> ] in canopy chloroplasts in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM	[C6a,C7b]	
$C_{c(64)}$	[CO <sub>2</sub> ] in C <sub>4</sub> bundle sheath	μM	[C38,C39,C42,C44,C45b]	
$C_{c(m4)}$	[CO <sub>2</sub> ] in C <sub>4</sub> mesophyll in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM	[C29,C30b,C39]	
$CF_i$	Clumping factor	-	[C1]	0.45 (needleleaf) 0.675 (broadleaf)
$C_i'$	[CO <sub>2</sub> ] in canopy leaves when $\psi_{ci} = 0$	μmol mol <sup>-1</sup>	[C5]	0.70 x $C_b$
$C_i$	[CO <sub>2</sub> ] in canopy leaves	μmol mol <sup>-1</sup>	[C2]	
$C_{i(m4)}'$	[CO <sub>2</sub> ] in C <sub>4</sub> mesophyll air when $\psi_{ci} = 0$	μmol mol <sup>-1</sup>	[C28]	0.45 x $C_b$
$C_{i(m4)}$	[CO <sub>2</sub> ] in C <sub>4</sub> mesophyll air	μmol mol <sup>-1</sup>	[C25]	
$C_{i,j,z=l}$	C content of leaf ( $z = l$ )	g C m <sup>-2</sup>	[C18a]	
$D_{e\ NH_4l}$	effective dispersivity-diffusivity of NH <sub>4</sub> <sup>+</sup> during root uptake	m <sup>2</sup> h <sup>-1</sup>	[C23]	
$D_{e\ NO_3l}$	effective dispersivity-diffusivity of NO <sub>3</sub> <sup>-</sup> during root uptake	m <sup>2</sup> h <sup>-1</sup>	[C23]	
$D_{e\ PO_4l}$	effective dispersivity-diffusivity of H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> during root uptake	m <sup>2</sup> h <sup>-1</sup>	[C23]	

$D_{r02}$	aqueous diffusivity of $O_2$ from root aerenchyma to root or mycorrhizal surfaces	$m^2 h^{-1}$	[C14d]		
$D_{s02}$	aqueous diffusivity of $O_2$ from soil to root or mycorrhizal surfaces	$m^2 h^{-1}$	[C14d]		
$d_{i,r,l}$	half distance between adjacent roots assumed equal to uptake path length	m	[C23]	$(\pi L_{s,z} / \Delta z)^{-1/2}$	Grant (1998)
$E_{N,P}$	energy cost of nutrient uptake	$g C g N^{-1}$ or $P^{-1}$	[C13]	2.15	Veen (1981)
$f_{C(c3)}$	$C_3$ product inhibition of RuBP carboxylation activity in $C_4$ bundle sheath or $C_3$ mesophyll	–	[C47,C48,C49]		
$f_{C(m4)}$	$C_4$ product inhibition of PEP carboxylation activity in $C_4$ mesophyll	–	[C32,C33,C34]		
$F_{chl}$	fraction of leaf protein in chlorophyll	–	[C8b]	0.025	
$f_{iC}$	N,P inhibition on carboxylation, leaf structural N,P growth	–	[C6a,C7,C11,C12]		
$f_{iN}$	N inhibition on root N uptake	–	[C23g]		
$f_{iP}$	P inhibition on root P uptake	–	[C23h]		
$f_{\lambda C}$	fraction of $X_{Cmx}$ translocated out of leaf or root before litterfall	–	[C18a,C19a]		
$f_{\lambda N}$	fraction of $X_N$ translocated out of leaf or root before litterfall	–	[C18b,C19b]		
$f_{\lambda P}$	fraction of $X_P$ translocated out of leaf or root before litterfall	–	[C18c,C19c]		
$F_{rubisco}$	fraction of leaf protein in rubisco	–	[C6b,d]	0.125	
$f_{ta}$	temperature effect on $R_{ai,j}$ and $U$	–	[C14,C22,C23]		
$f_{tb}$	temperature effect on carboxylation	–	[C6b,C10a]		
$f_{tj}$	temperature effect on electron transport		[C8b,C10c]		

$f_{tkc}$	temperature effect on $K_{c_i}$		[C6e,C10d]	Bernacchi et al. (2001,2003)
$f_{tko}$	temperature effect on $K_{o_i}$		[C6e,C10e]	Bernacchi et al. (2001,2003)
$f_{tm}$	temperature effect on $R_{mi,j}$	–	[C16, C22b]	$Q_{10} = 2.25$
$f_{to}$	temperature effect on oxygenation		[C6d,C10b]	
$f_{tv}$	temperature effect on carboxylation	–	[C32,C33,C36,C47,C48]	
$f_{xN}$	inhibition of root or mycorrhizal N exudation	–	[C19e,g]	
$f_{xP}$	inhibition of root or mycorrhizal P exudation	–	[C19f,h]	
$f_{\psi i}$	non-stomatal water effect on carboxylation	–	[C6a,C7a,C9]	Medrano et al. (2002)
$f_{\psi i}$	non-stomatal water effect on carboxylation	–	[C32,C33,C35C47,C48]	
$g_{sC}$	conductance for shoot-root C transfer	$h^{-1}$	[C50]	calculated from root depth, axis number
$g_{sN,P}$	rate constant for shoot-root N,P transfer	$h^{-1}$	[C51]	0.1
$g_{rC}$	rate constant for root-mycorrhizal C transfer	$h^{-1}$	[C52]	0.1
$g_{rN,P}$	rate constant for root-mycorrhizal N,P transfer	$h^{-1}$	[C53]	0.1
$H_{aj}$	energy of activation for electron transport	$J \text{ mol}^{-1}$	[C10c]	$43 \times 10^3$
$H_{akc}$	parameter for temperature sensitivity of $K_{c_i}$	$J \text{ mol}^{-1}$	[C10d]	$55 \times 10^3$
$H_{ako}$	parameter for temperature sensitivity of $K_{o_i}$	$J \text{ mol}^{-1}$	[C10e]	$20 \times 10^3$
$H_{ao}$	energy of activation for oxygenation	$J \text{ mol}^{-1}$	[C10b, C22]	$60 \times 10^3$

$H_{av}$	energy of activation for carboxylation	$\text{J mol}^{-1}$	[C10a, C22]	$65 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{dh}$	energy of high temperature deactivation	$\text{J mol}^{-1}$	[C10, C22]	$222.5 \times 10^3$	
$H_{dl}$	energy of low temperature deactivation	$\text{J mol}^{-1}$	[C10, C22]	$197.5 \times 10^3$	
$[\text{H}_2\text{PO}_4^-]_{i,r,l}$	concentration of $\text{H}_2\text{PO}_4^-$ root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[C23]		
$[\text{H}_2\text{PO}_4^-]_{mn}$	concentration of $\text{H}_2\text{PO}_4^-$ at root or mycorrhizal surfaces below which $U_{\text{PO}_4} = 0$	$\text{g N m}^{-3}$	[C23]	0.002	Barber and Silberbush, 1984
$I$	irradiance	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C8a,]		
$J$	electron transport rate in $\text{C}_3$ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C7a,C8a]		
$J_{(b4)}$	electron transport rate in $\text{C}_4$ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C45a,C46]		
$J_{(m4)}$	electron transport rate in $\text{C}_4$ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C30a,C31]		
$J_{\max}'$	specific electron transport rate at non-limiting $I$ and $25^\circ\text{C}$ when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{s}^{-1}$	[C33,C48]	400	
$J_{\max(b4)}$	electron transport rate in $\text{C}_4$ bundle sheath at non-limiting $I$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C46,C48]		
$J_{\max(m4)}$	electron transport rate in $\text{C}_4$ mesophyll at non-limiting $I$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C31,C33]		
$J_{\max}$	electron transport rate at non-limiting $I$ , $\psi_{ci}$ , temperature and N,P	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C8a,C8b]		
$K_{c(b4)}$	Michaelis-Menten constant for carboxylation in $\text{C}_4$ bundle sheath	$\mu\text{M}$	[C44]	30.0 at $25^\circ\text{C}$ and zero $\text{O}_2$	Lawlor (1993)
$K_{c(m4)}$	Michaelis-Menten constant for carboxylation in $\text{C}_4$ mesophyll	$\mu\text{M}$	[C29]	3.0 at $25^\circ\text{C}$	Lawlor (1993)
$K_c$	Michaelis-Menten constant for carboxylation at zero $\text{O}_2$	$\mu\text{M}$	[C6c,C6e]	12.5 at $25^\circ\text{C}$	Farquhar et al. (1980)
$K_c$	Michaelis-Menten constant for carboxylation at ambient $\text{O}_2$	$\mu\text{M}$	[C6e]		
$K_{iCN}$	inhibition constant for growth in shoots from $\sigma_C$ vs. $\sigma_N$	$\text{g C g N}^{-1}$	[C11]	100	Grant (1998)

$K_{iC_P}$	inhibition constant for growth in shoots from $\sigma_C$ vs. $\sigma_P$	g C g P <sup>-1</sup>	[C11]	1000	Grant (1998)
$K_{I_{\chi C4(b4)}}$	constant for CO <sub>2</sub> product inhibition of C <sub>4</sub> decarboxylation in C <sub>4</sub> bundle sheath	μM	[C38]	1000	
$K_{I_{\chi C4(m4)}}$	constant for C <sub>4</sub> product inhibition of PEP carboxylation activity in C <sub>4</sub> mesophyll	μM	[C34]	5 x 10 <sup>6</sup>	
$K_{I_{vlf}}$	constant for C <sub>3</sub> product inhibition of RuBP carboxylation activity in C <sub>4</sub> bundle sheath or C <sub>3</sub> mesophyll caused by $[V_{fij}]$	g C g N <sup>-1</sup>	[C49]	100	
$K_{I_{rlf}}$	constant for C <sub>3</sub> product inhibition of RuBP carboxylation activity in C <sub>4</sub> bundle sheath or C <sub>3</sub> mesophyll caused by $[\pi_{fij}]$	g C g P <sup>-1</sup>	[C49]	1000	
$K_{iN_C}$	inhibition constant for N uptake in roots from $\sigma_{C_{i,j}}$ vs. $\sigma_{N_j}$	g N g C <sup>-1</sup>	[C23]	0.1	Grant (1998)
$K_{iP_C}$	inhibition constant for P uptake in roots from $\sigma_{C_{i,j}}$ vs. $\sigma_{P_{i,j}}$ roots	g P g C <sup>-1</sup>	[C23]	0.01	Grant (1998)
$K_{\lambda N}$	constant used to calculate remobilization of leaf or root C and N during senescence	g N g C <sup>-1</sup>	[C19a,C19b]	0.1	
$K_{\lambda P}$	constant used to calculate remobilization of leaf or root C and P during senescence	g P g C <sup>-1</sup>	[C19a,C19c]	0.01	
$K_{NH_4}$	M-M constant for NH <sub>4</sub> <sup>+</sup> uptake at root or mycorrhizal surfaces	g N m <sup>-3</sup>	[C23]	0.40	Barber and Silberbush, 1984
$K_{NO_3}$	M-M constant for NO <sub>3</sub> <sup>-</sup> uptake at root or mycorrhizal surfaces	g N m <sup>-3</sup>	[C23]	0.35	Barber and Silberbush, 1984
$K_{PO_4}$	M-M constant for H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> uptake root or mycorrhizal surfaces	g P m <sup>-3</sup>	[C23]	0.125	Barber and Silberbush, 1984
$K_{O_2}$	Michaelis-Menten constant for root or mycorrhizal O <sub>2</sub> uptake	g m <sup>-3</sup>	[C14c]	0.32	Griffin (1972)
$K_o$	inhibition constant for O <sub>2</sub> in carboxylation	μM	[C6c,C6e]	500 at 25 °C	Farquhar et al. (1980)
$K_{xN}$	inhibition constant for exudation of root or mycorrhizal N	g C g N <sup>-1</sup>	[C19g]	1.0	
$K_{xP}$	inhibition constant for exudation of root or mycorrhizal P	g C g N <sup>-1</sup>	[C19h]	10.0	

$L$	root length	$\text{m m}^{-2}$	[C14d,C21b,C23]	
$l_C$	C litterfall from leaf or root	$\text{g C m}^{-2} \text{ h}^{-1}$	[C18a,C18b,C18c, C20]	
$l_N$	N litterfall from leaf or root	$\text{g C m}^{-2} \text{ h}^{-1}$	[C18b]	
$l_P$	P litterfall from leaf or root	$\text{g C m}^{-2} \text{ h}^{-1}$	[C18c]	
$M_L$	leaf C phytomass	$\text{g C m}^{-2}$	[C12,C21]	
$M_{L_N}, M_{L_R}$	non-remobilizable, remobilizable (protein) leaf C phytomass	$\text{g C m}^{-2}$	[C12,C18a]	
$M_M$	mycorrhizal C phytomass	$\text{g C m}^{-2}$	[C52]	
$M_R$	root C phytomass	$\text{g C m}^{-2}$	[C20,C21,C50,C5 2]	
$M_{L_iprot}$	leaf protein phytomass calculated from leaf N, P contents	$\text{g N m}^{-2}$	[C6b,C6d,C8b]	
$N, P$	N or P content of organ $z$	$\text{g N m}^{-2}$	[C16, C19]	
$N_{leaf}$	maximum leaf structural N content	$\text{g N g C}^{-1}$	[C12]	0.10
$N'_{leaf}$	minimum leaf structural N content	$\text{g N g C}^{-1}$	[C12]	$0.33 \times N_{leaf}$
$N_{lf}$	total leaf N	$\text{g N m}^{-2} \text{ leaf}$	[C32,C33,C47,C4 8]	
$N_{prot}$	N content of protein remobilized from leaf or root	$\text{g N C}^{-1}$	[C12,C18b]	0.4
$[N_{chl(b4)}]'$	ratio of chlorophyll N in $C_4$ bundle sheath to total leaf N	$\text{g N g N}^{-1}$	[C48]	0.05
$[N_{chl(m4)}]'$	ratio of chlorophyll N in $C_4$ mesophyll to total leaf N	$\text{g N g N}^{-1}$	[C33]	0.05
$[\text{NH}_4^+_{i,r,l}]$	concentration of $\text{NH}_4^+$ at root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[C23]	
$[\text{NH}_4^+_{mn}]$	concentration of $\text{NH}_4^+$ at root or mycorrhizal surfaces below which $U_{\text{NH}_4} = 0$	$\text{g N m}^{-3}$	[C23]	0.0125
$[\text{NO}_3^-_{i,r,l}]$	concentration of $\text{NH}_4^+$ at root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[C23]	Barber and Silberbush, 1984

$[\text{NO}_3^-]_{\text{mn}}$	concentration of $\text{NO}_3^-$ at root or mycorrhizal surfaces below which $U_{\text{NO}_3} = 0$	$\text{g N m}^{-3}$	[C23]	0.03	Barber and Silberbush, 1984
$[N_{\text{pep(m4)}}]'$	ratio of PEP carboxylase N in $\text{C}_4$ mesophyll to total leaf N	$\text{g N g N}^{-1}$	[C32]	0.025	
$[N_{\text{rub(b4)}}]'$	ratio of RuBP carboxylase N in $\text{C}_4$ bundle sheath to total leaf N	$\text{g N g N}^{-1}$	[C47]	0.025	
$O_{2q}$	aqueous $\text{O}_2$ concentration in root or mycorrhizal aerenchyma	$\text{g m}^{-3}$	[C14c,d]		
$O_{2r}$	aqueous $\text{O}_2$ concentration at root or mycorrhizal surfaces	$\text{g m}^{-3}$	[C14c,d]		
$O_{2s}$	aqueous $\text{O}_2$ concentration in soil solution	$\text{g m}^{-3}$	[C14c,d]		
$O_c$	$[\text{O}_2]$ in canopy chloroplasts in equilibrium with $\text{O}_2$ in atm.	$\mu\text{M}$	[C6c,C6e]		
$P_{\text{leaf}}$	maximum leaf structural P content	$\text{g P g C}^{-1}$	[C12]	0.10	
$P'_{\text{leaf}}$	minimum leaf structural P content	$\text{g P g C}^{-1}$	[C12]	$0.33 \times P_{\text{leaf}}$	
$P_{\text{prot}}$	P content of protein remobilized from leaf or root	$\text{g P C}^{-1}$	[C12,C18c]	0.04	
$[\pi_{\text{lf}}]$	concentration of nonstructural root P uptake product in leaf	$\text{g P g C}^{-1}$	[C49]		
$\theta_P$	root or mycorrhizal porosity	$\text{m}^3 \text{ m}^{-3}$	[C21b]	0.1 – 0.5	
$R$	gas constant	$\text{J mol}^{-1} \text{ K}^{-1}$	[C10, C22]	8.3143	
$R_a$	total autotrophic respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13]		
$R'_a$	$R_a$ under nonlimiting $\text{O}_2$	$\text{g C m}^{-2} \text{ h}^{-1}$	[C14]		
$R'_c$	specific autotrophic respiration of $\sigma_{\text{C}_{i,j}}$ at $T_{ci} = 25^\circ\text{C}$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[C14]	0.015	
$R_c$	autotrophic respiration of $\sigma_{\text{C}_{i,j}}$ or $\sigma_{\text{C}_{i,r,l}}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13,C14,C17, C15]		
$R_g$	growth respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C17,C20]		
$r_{\text{lf}}$	leaf stomatal resistance	$\text{s m}^{-1}$	[C25,C27,C39]		

$r_{lfmaxi}$	leaf cuticular resistance	$\text{s m}^{-1}$	[C27]		
$r_{lfmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	$\text{s m}^{-1}$	[C27,C28,C35]		
$r_{li,j,k,l,m,n,o}$	leaf stomatal resistance	$\text{s m}^{-1}$	[C2,C4,C9]		
$r_{lmaxi}$	leaf cuticular resistance	$\text{s m}^{-1}$	[C4]		
$r_{lmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	$\text{s m}^{-1}$	[C4,C5,C9]		
$R_m'$	specific maintenance respiration of $\sigma_{Cij}$ at $T_{ci} = 25^\circ\text{C}$	$\text{g C g N}^{-1} \text{ h}^{-1}$	[C16]	0.0115	Barnes et al. (1998)
$R_{mi,j}$	above-ground maintenance respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C16,C17,C15]		
$r_{qi,r,l}$	radius of root aerenchyma	$\text{m}$	[C14d]		
$r_{ri,r,l}$	root or mycorrhizal radius	$\text{m}$	[C14d,C21b,c,C23 a,c,e]	$1.0 \times 10^{-4}$ or $5.0 \times 10^{-6}$	
$R_{si,j}$	respiration from remobilization of leaf C	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13,C15,C18a, C20]		
$r_{sl}$	thickness of soil water films	$\text{m}$	[C14d]		
$r_x$	rate constant for root or mycorrhizal exudation	$\text{h}^{-1}$	[C19d,e,f]	0.001	
$\rho_r$	dry matter content of root biomass	$\text{g g}^{-1}$	[C21b]	0.125	
$S$	change in entropy	$\text{J mol}^{-1} \text{ K}^{-1}$	[C10, C22]	710	Sharpe and DeMichelle (1977)
$\sigma_C$	nonstructural C product of $\text{CO}_2$ fixation	$\text{g C g C}^{-1}$	[C11,C19,C23g,h, C50-53]		
$\sigma_N$	nonstructural N product of root uptake	$\text{g N g C}^{-1}$	[C11,C19,C23g,h, C51,C53]		
$\sigma_P$	nonstructural P product of root uptake	$\text{g P g C}^{-1}$	[C11,C19,C23g,h, C51,C53]		

$T_c$	canopy temperature	K	[C10, C22]		
$U_{\text{NH4}i,r,l}$	$\text{NH}_4^+$ uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
$U'_{\text{NH}_4}$	maximum $U_{\text{NH}_4}$ at 25 °C and non-limiting $\text{NH}_4^+$	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	$5.0 \times 10^{-3}$	Barber and Silberbush, 1984
$U_{\text{NO}_3i,r,l}$	$\text{NO}_3^-$ uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
$U'_{\text{NO}_3}$	maximum $U_{\text{NO}_3}$ at 25 °C and non-limiting $\text{NO}_3^-$	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	$5.0 \times 10^{-3}$	Barber and Silberbush, 1984
$U_{\text{PO}_4i,r,l}$	$\text{H}_2\text{PO}_4^-$ uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
$U'_{\text{PO}_4}$	maximum $U_{\text{PO}_4}$ at 25 °C and non-limiting $\text{H}_2\text{PO}_4^-$	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	$5.0 \times 10^{-3}$	Barber and Silberbush, 1984
$U_{\text{O}_2i,r,l}$	$\text{O}_2$ uptake by roots and mycorrhizae under ambient $\text{O}_2$	$\text{g O m}^{-2} \text{ h}^{-1}$	[C14b,c,C23b,d,f]		
$U'_{\text{O}_2i,l,r}$	$\text{O}_2$ uptake by roots and mycorrhizae under nonlimiting $\text{O}_2$	$\text{g O m}^{-2} \text{ h}^{-1}$	[C14b,c,C23b,d,f]		
$U_{\text{w},i,r,l}$	root water uptake	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[C14d,C23]		
$V_{\text{d}(\text{b}4)i,j,k}$	$\text{CO}_2$ leakage from $\text{C}_4$ bundle sheath to $\text{C}_4$ mesophyll	$\text{g C m}^{-2} \text{ h}^{-1}$	[C39,C42]		
$V_b'$	specific rubisco carboxylation at 25 °C	$\mu\text{mol g}^{-1} \text{ rubisco s}^{-1}$	[C6b]	45	Farquhar et al. (1980)
$V_{\text{b}(\text{b}4)i,j,k}$	$\text{CO}_2$ -limited carboxylation rate in $\text{C}_4$ bundle sheath	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C43,C44]		
$V_{\text{b}(\text{m}4)i,j,k,l,m,n,o}$	$\text{CO}_2$ -limited carboxylation rate in $\text{C}_4$ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C26]		
$V_{\text{bi},j,k,l,m,n,o}$	$\text{CO}_2$ -limited leaf carboxylation rate	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C3,C6]		
$V_{\text{bmax}(\text{b}4)}'$	RuBP carboxylase specific activity in $\text{C}_4$ bundle sheath at 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{ s}^{-1}$	[C47]	75	
$V_{\text{bmax}(\text{b}4)i,j,k}$	$\text{CO}_2$ -nonlimited carboxylation rate in $\text{C}_4$ bundle sheath	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C44,C47]		
$V_{\text{bmax}(\text{m}4)}'$	PEP carboxylase specific activity in $\text{C}_4$ mesophyll at 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{ s}^{-1}$	[C32]	150	

$V_{b\max(m4)i,j,k}$	CO <sub>2</sub> -nonlimited carboxylation rate in C <sub>4</sub> mesophyll	μmol m <sup>-2</sup> s <sup>-1</sup>	[C29,C32]	
$V_{b\max i,j,k}$	leaf carboxylation rate at non-limiting CO <sub>2</sub> , $\psi_{ci}$ , $T_c$ and N,P	μmol m <sup>-2</sup> s <sup>-1</sup>	[C6a,C6b,C6c]	
$V_{c(b4)i,j,k,l,m,n,o}$	CO <sub>2</sub> fixation rate in C <sub>4</sub> bundle sheath	μmol m <sup>-2</sup> s <sup>-1</sup>	[C43]	
$V_{c(m4)i,j,k,l,m,n,o}$	CO <sub>2</sub> fixation rate in C <sub>4</sub> mesophyll	μmol m <sup>-2</sup> s <sup>-1</sup>	[C24,C26,C40,C41]	
$V_{c0(m4)i,j,k,l,m,n,o}$	CO <sub>2</sub> fixation rate in C <sub>4</sub> mesophyll when $\psi_{ci} = 0$ MPa	μmol m <sup>-2</sup> s <sup>-1</sup>	[C28]	
$V_{ci,j,k,l,m,n,o}$	leaf CO <sub>2</sub> fixation rate	μmol m <sup>-2</sup> s <sup>-1</sup>	[C1,C3]	
$V_{c'}_{i,j,k,l,m,n,o}$	leaf CO <sub>2</sub> fixation rate when $\psi_{ci} = 0$	μmol m <sup>-2</sup> s <sup>-1</sup>	[C5]	
$V_{g(m4)i,j,k,l,m,n,o}$	CO <sub>2</sub> diffusion rate into C <sub>4</sub> mesophyll	μmol m <sup>-2</sup> s <sup>-1</sup>	[C24,C25]	
$V_{gi,j,k,l,m,n,o}$	leaf CO <sub>2</sub> diffusion rate	μmol m <sup>-2</sup> s <sup>-1</sup>	[C1,C2]	
$V_j'$	specific chlorophyll e <sup>-</sup> transfer at 25 °C	μmol g <sup>-1</sup> chlorophyll s <sup>-1</sup>	[C8b]	450
				Farquhar et al. (1980)
$V_{j(b4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C <sub>4</sub> bundle sheath	μmol m <sup>-2</sup> s <sup>-1</sup>	[C43,C45a]	
$V_{j(m4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C <sub>4</sub> mesophyll	μmol m <sup>-2</sup> s <sup>-1</sup>	[C26,C30a]	
$V_{ji,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	μmol m <sup>-2</sup> s <sup>-1</sup>	[C3,C7a]	
$V_o'$	specific rubisco oxygenation at 25 °C	μmol g <sup>-1</sup> rubisco s <sup>-1</sup>	[C6d]	9.5
				Farquhar et al. (1980)
$V_{o\max i,j,k}$	leaf oxygenation rate at non-limiting O <sub>2</sub> , $\psi_{ci}$ , $T_c$ and N,P	μmol m <sup>-2</sup> s <sup>-1</sup>	[C6c,d]	
$V_{\chi C4(b4)i,j,k}$	decarboxylation of C <sub>4</sub> fixation product in C <sub>4</sub> bundle sheath	g C m <sup>-2</sup> h <sup>-1</sup>	[C38,C41,C42]	
$V_{\chi C4(m4)}$	transfer of C <sub>4</sub> fixation product between C <sub>4</sub> mesophyll and bundle sheath	g C m <sup>-2</sup> h <sup>-1</sup>	[C37]	
[ $v_{lf}$ ]	concentration of nonstructural root N uptake product in leaf	g N g C <sup>-1</sup>	[C49]	

$v_r$	specific volume of root biomass	$\text{m}^3 \text{ g}^{-1}$	[C21b]	
$W_{\text{lf(b4)}}$	$\text{C}_4$ bundle sheath water content	$\text{g m}^{-2}$	[C37,C39]	
$W_{\text{lf(m4)}}$	$\text{C}_4$ mesophyll water content	$\text{g m}^{-2}$	[C37]	
$X_{\text{Cmn}}$	minimum fraction of remobilizable C translocated out of leaf or root during senescence	-	[C18a]	0.167 Kimmins (2004)
$X_{\text{Cmx}}$	maximum fraction of remobilizable C translocated out of leaf or root during senescence	-	[C18a]	0.50 Kimmins (2004)
$X_{\text{N,P}}$	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	[C18b,C18c]	0.8 Kimmins (2004)
$x_{i,r,l,C}$	root and mycorrhizal C exudation	$\text{g C m}^{-2} \text{ h}^{-1}$	[C19d]	
$x_{i,r,l,N}$	root and mycorrhizal C exudation	$\text{g N m}^{-2} \text{ h}^{-1}$	[C19e]	
$x_{i,r,l,P}$	root and mycorrhizal C exudation	$\text{g P m}^{-2} \text{ h}^{-1}$	[C19f]	
$Y$	carboxylation yield from electron transport in $\text{C}_3$ mesophyll	$\mu\text{mol CO}_2 \mu\text{mol e}^{-}$	[C7a,b]	
$Y_{\text{(b4)}}$	carboxylation yield from electron transport in $\text{C}_4$ bundle sheath	$\mu\text{mol CO}_2 \mu\text{mol e}^{-}$	[C45a,b]	
$Y_{\text{(m4)}}$	carboxylation yield from electron transport in $\text{C}_4$ mesophyll	$\mu\text{mol CO}_2 \mu\text{mol e}^{-}$	[C30a,b]	
$Y_g$	fraction of $\sigma_{\text{C}i,j}$ used for growth expended as $R_{gi,j,z}$ by organ $z$	$\text{g C g C}^{-1}$	[C20]	0.28 ( $z = \text{leaf}$ ), 0.24 ( $z = \text{root and other non-foliar}$ ), 0.20 ( $z = \text{wood}$ ) Waring and Running (1998)
$y$	plant population	$\text{m}^{-2}$	[C21]	
$Z_{sC}$	shoot-root C transfer	$\text{g C m}^{-2} \text{ h}^{-1}$	[C50]	

$Z_{sN,P}$	shoot-root N,P transfer	$\text{g N,P m}^{-2} \text{h}^{-1}$	[C51]	
$Z_{rC}$	root-mycorrhizal C transfer	$\text{g C m}^{-2} \text{h}^{-1}$	[C52]	
$Z_{rN,P}$	root-mycorrhizal N,P transfer	$\text{g N,P m}^{-2} \text{h}^{-1}$	[C53]	
$\Gamma$	$\text{CO}_2$ compensation point in $\text{C}_3$ mesophyll	$\mu\text{M}$	[C6a,C6c,C7b]	
$\Gamma_{(\text{b4})}$	$\text{CO}_2$ compensation point in $\text{C}_4$ bundle sheath	$\mu\text{M}$	[C44,C45b]	
$\Gamma_{(\text{m4})}$	$\text{CO}_2$ compensation point in $\text{C}_4$ mesophyll	$\mu\text{M}$	[C29,C30b]	
$\alpha$	shape parameter for response of $J$ to $I$	-	[C8a]	0.7
$\alpha$	shape parameter for response of $J$ to $I$	-	[C31,C46]	0.75
$\chi$	area:mass ratio of leaf growth	$\text{m g}^{-3}$	[C21]	0.0125
				Grant and Hesketh (1992)
$\chi_{\text{C4(b4)}}$	non-structural $\text{C}_4$ fixation product in $\text{C}_4$ bundle sheath	$\text{g C m}^{-2}$	[C37,C38,C41]	
$\chi_{\text{C4(m4)}}$	non-structural $\text{C}_4$ fixation product in $\text{C}_4$ mesophyll	$\text{g C m}^{-2}$	[C37,C40]	
$[\chi_{\text{c3(b4)}}]$	concentration of non-structural $\text{C}_3$ fixation product in $\text{C}_4$ bundle sheath	$\text{g g}^{-1}$	[C49]	
$[\chi_{\text{C4(m4)}}]$	concentration of non-structural $\text{C}_4$ fixation product in $\text{C}_4$ mesophyll	$\mu\text{M}$	[C34]	
$\varepsilon$	quantum yield	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[C8a]	0.45
$\varepsilon$	quantum yield	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[C31,C46]	0.45
				Farquhar et al. (1980)
$\kappa_{\text{Cc(b4)}}$	conductance to $\text{CO}_2$ leakage from $\text{C}_4$ bundle sheath	$\text{h}^{-1}$	[C39]	20
$\psi_t$	canopy turgor potential	$\text{MPa}$	[C4]	1.25 at $\psi_c = 0$

## **S4: Soil Water, Heat, Gas and Solute Fluxes**

### *Surface Water Flux*

Surface runoff is modelled using Manning's equation [D1a] with surface water velocity  $v$  [D3] calculated from surface geometry [D5a] and slope [D5b], and with surface water depth  $d$  [D2] calculated from surface water balance [D4] using kinematic wave theory. Lateral snow transfer is modelled from elevational differences between snowpack surfaces in adjacent grid cells such that over time these surfaces approach a common elevation across a landscape [D1b].

### *Subsurface Water Flux*

Subsurface water flow [D7] is calculated from Richard's equation using bulk soil water potentials  $\psi_s$  of both cells if both source and destination cells are unsaturated [D9a], or Green-Ampt equation using  $\psi_s$  beyond the wetting front of the unsaturated cell if either source or destination cell is saturated [D9b] (Grant et al., 2004). Subsurface water flow can also occur through macropores using Poiseulle-Hagen theory for laminar flow in tubes (Dimitrov et al., 2010), depending on inputs for macropore volume fraction.

### *Exchange with Water Table*

If a water table is present in the model, subsurface boundary water fluxes between saturated boundary grid cells and a fixed external water table are calculated from lateral hydraulic conductivities of the grid cells, and from elevation differences and lateral distances between the grid cells and the external water table [D10]. These terms are determined from set values for the depth  $d_t$  of, and lateral distance  $L_t$  to, an external water table.

### *Surface Heat Flux*

Surface heat fluxes ( $G$ ) arising from closure of the energy balance at snowpack, surface litter and soil surfaces [D11] (Grant et al., 1999) drive conductive – convective fluxes among snowpack, surface litter and soil layers [D12]. These fluxes drive freezing – thawing ( $Q_f$ ) and changes temperatures ( $T$ ) in snowpack, surface litter and soil layers [D13].

### *Gas Flux*

All gases undergo volatilization – dissolution between the gaseous and aqueous phases in the soil [D14a] and root [D14b], and between the atmosphere and the aqueous phase at the soil surface [D15a], driven by gaseous – aqueous concentration differences calculated from solubility coefficients and coupled to diffusive uptake by roots [C14] and microbes [A17]. Gases also undergo convective - conductive transfer among soil layers driven by gaseous concentration gradients and diffusivities [D16a,b,c] calculated from air-filled porosities [D17a,b,c], and from each rooted soil layer directly to the atmosphere through roots driven by gaseous

concentration gradients and diffusivities [D16d] calculated from root porosities [D17d]. Gases may also bubble upwards from soil zones in which the total partial pressure of all aqueous gases exceeds atmospheric pressure [D18].

#### *Solute Flux*

All gaseous and non-gaseous solutes undergo convective - dispersive transfer among soil layers and through roots in each soil layer driven by aqueous concentration gradients and dispersivities [D19] calculated from water-filled porosity [D20] and water flow length [D21].

**Table S4: Soil Water, Heat, Gas and Solute Fluxes**

<i>Surface Water Flux</i>	
$Q_{rx(x,y)} = v_{x(x,y)} d_{mx,y} L_{y(x,y)}$	lateral water transfer from 2D Manning equation in $x$ (EW) and $y$ (NS) directions [D1a]
$Q_{(s,w,i)x(x,y)} = (2 F [(Z_{x,y} + z_{sx,y}) - (Z_{x+1,y} + z_{sx+1,y})] / (L_{x(x,y)} + L_{x(x+1,y)})) V_{(s,w,i)}$	topographically-driven snowpack snow $s$ , water $w$ and ice $i$ transfer in $x$ (EW) and $y$ (NS) directions [D1b]
$Q_{(s,w,i)y(x,y)} = (2 F [(Z_{x,y} + z_{sx,y}) - (Z_{x,y+1} + z_{sx,y+1})] / (L_{x(x,y)} + L_{x(x,y+1)})) V_{(s,w,i)}$	
$d_{x,y} = \max(0, d_{w(x,y)} + d_{i(x,y)} - d_{s(x,y)}) d_{w(x,y)} / (d_{w(x,y)} + d_{i(x,y)})$	surface water depth [D2]
$v_{x(x,y)} = R^{0.67} s_{x(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over E slope [D3]
$v_{y(x,y)} = R^{0.67} s_{y(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over S slope
$v_{x(x,y)} = -R^{0.67} s_{x(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over W slope
$v_{y(x,y)} = -R^{0.67} s_{y(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over N slope
$\Delta(d_{w(x,y)} A_{x,y}) / \Delta t = Q_{r,x(x,y)} - Q_{r,x+1(x,y)} + Q_{r,y(x,y)} - Q_{r,y+1(x,y)} + P - E_{x,y} - Q_{wz(x,y,I)}$	2D kinematic wave theory for overland flow [D4]
$R = s_r d_m / [2 (s_r^2 + 1) 0.5]$	wetted perimeter [D5a]
$s_{x(x,y)} = 2 \text{abs}[(Z_{x,y} + d_{sx,y} + d_{mx,y}) - (Z_{x+1,y} + d_{sx+1,y} + d_{mx+1,y})] / (L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and pooled surface water in $x$ (EW) and $y$ (NS) directions [D5b]
$s_{y(x,y)} = 2 \text{abs}[(Z_{x,y} + d_{sx,y} + d_{mx,y}) - (Z_{x,y+1} + d_{sx,y+1} + d_{mx,y+1})] / (L_{y(x,y)} + L_{y(x,y+1)})$	
$LE_l = L (e_a - e_{l(T_l, \psi_l)}) / r_{al}$	evaporation from surface litter [D6a]
$LE_s = L (e_a - e_{s(T_s, \psi_s)}) / r_{as}$	evaporation from soil surface [D6b]

*Subsurface Water Flux*

$$Q_{wx(x,y,z)} = K'_x (\psi_{sx,y,z} - \psi_{sx+I,y,z})$$

$$Q_{wy(x,y,z)} = K'_y (\psi_{sx,y,z} - \psi_{sx,y+I,z})$$

$$Q_{wz(x,y,z)} = K'_z (\psi_{sx,y,z} - \psi_{sx,y,z+I})$$

$$\begin{aligned} \psi_m(\theta) &= -\exp [ \ln(-\psi_{FC}) + \{ (\ln\theta_{FC} - \ln\theta) / (\ln\theta_{FC} - \ln\theta_{WP}) * (\ln(-\psi_{FC}) - \ln(-\psi_{WP})) \} ] \quad (\theta < \theta_{FC}) \\ &= -\exp [ \ln(-\psi_{ST}) + \{ (\ln\theta_{ST} - \ln\theta) / (\ln\theta_{ST} - \ln\theta_{FC}) * (\ln(-\psi_{ST}) - \ln(-\psi_{FC})) \} ] \quad (\theta \geq \theta_{FC}) \end{aligned}$$

$$\psi_s = \psi_m + \psi_\pi + \psi_g$$

$$\Delta\theta_{w,x,y,z}/\Delta t = (Q_{wx(x,y)} - Q_{wx+I(x,y)} + Q_{wy(x,y)} - Q_{wy+I(x,y)} + Q_{wz(x,y)} - Q_{wz+I(x,y)} + Q_{f(x,y,z)}) / L_{z(x,y,z)}$$

$$K'_x = 2 K_{x,y,z} K_{x+I,y,z} / (K_{x,y,z} L_{x,(x+I,y,z)} + K_{x+I,y,z} L_{x,(x,y,z)})$$

$$= 2 K_{x,y,z} / (L_{x(x+I,y,z)} + L_{x(x,y,z)})$$

$$= 2 K_{x+I,y,z} / (L_{x(x+I,y,z)} + L_{x(x,y,z)})$$

$$K'_y = 2 K_{x,y,z} K_{x,y+I,z} / (K_{x,y,z} L_{y(x,y+I,z)} + K_{x,y+I,z} L_{y(x,y,z)})$$

$$= 2 K_{x,y,z} / (L_{y(x,y+I,z)} + L_{y(x,y,z)})$$

$$= 2 K_{x,y+I,z} / (L_{y(x,y+I,z)} + L_{y(x,y,z)})$$

$$K'_z = 2 K_{x,y,z} K_{x,y,z+I} / (K_{x,y,z} L_{z(x,y,z+I)} + K_{x,y,z+I} L_{z(x,y,z)})$$

$$= 2 K_{x,y,z} / (L_{z(x,y,z+I)} + L_{z(x,y,z)})$$

$$= 2 K_{x,y,z+I} / (L_{z(x,y,z+I)} + L_{z(x,y,z)})$$

3D Richard's or Green-Ampt equation depending on saturation of source or target cell in  $x$  (EW),  $y$  (NS) and  $z$  (vertical) directions

[D7a]

[D7b]

[D7c]

matric water potential from water content

[D7d]

total soil water potential

[D7e]

3D water transfer plus freeze-thaw

[D8]

in direction  $x$  if source and destination cells are unsaturated

[D9a]

in direction  $x$  if source cell is saturated

[D9b]

in direction  $x$  if destination cell is saturated

[D9c]

in direction  $y$  if source and destination cells are unsaturated

[D9a]

in direction  $y$  if source cell is saturated

[D9b]

in direction  $y$  if destination cell is saturated

[D9c]

in direction  $z$  if source and destination cells are unsaturated

[D9a]

in direction  $z$  if source cell is saturated

[D9b]

in direction  $z$  if destination cell is saturated

[D9c]

### Exchange with Water Table

$$Q_{tx(x,y,z)} = K_{x,y,z} [\psi' - \psi_{sx,y,z} + 0.01 (d_{zx,y,z} - d_t)] / (L_{tx} + 0.5 L_{x,(x,y,z)})$$

if  $\psi_{sx,y,z} > \psi' + 0.01(d_{zx,y,z} - d_t)$  in

[D10]

$$Q_{\text{ty}(x,y,z)} = K_{x,y,z} [\psi' - \psi_{s,x,y,z} + 0.01 (d_{zx,y,z} - d_t)] / (L_{\text{ty}} + 0.5 L_{y,(x,y,z)})$$

$x$  (EW) and  $y$  (NS) directions for all depths  $z$  from  $d_{zx,y,z}$  to  $d_t$  or if  $d_{zx,y,z} > d_t$

### Heat Flux

$$R_n + LE + H + G = 0$$

$$G_{x(x,y,z)} = 2 \kappa_{(x,y,z),(x+I,y,z)} (T_{(x,y,z)} - T_{(x+I,y,z)}) / (L_{x(x,y,z)} + L_{x(x+I,y,z)}) + c_w T_{(x,y,z)} Q_{wx(x,y,z)}$$

$$G_{y(x,y,z)} = 2 \kappa_{(x,y,z),(x,y+I,z)} (T_{(x,y,z)} - T_{(x,y+I,z)}) / (L_{y(x,y,z)} + L_{y(x,y+I,z)}) + c_w T_{(x,y,z)} Q_{wy(x,y,z)}$$

$$G_{z(x,y,z)} = 2 \kappa_{(x,y,z),(x,y,z+I)} (T_{(x,y,z)} - T_{(x,y,z+I)}) / (L_{z(x,y,z)} + L_{z(x,y,z+I)}) + c_w T_{(x,y,z)} Q_{wz(x,y,z)}$$

for each canopy, snow, residue and soil surface, depending on exposure

[D11]

3D conductive – convective heat flux among snowpack, surface

[D12a]

residue and soil layers in  $x$  (EW),  $y$  (NS) and  $z$  (vertical) directions

[D12b]

[D12c]

$$\begin{aligned} \kappa_{(x,y,z)} = & (W_{o(x,y,z)} V_{o(x,y,z)} \kappa'_{o(x,y,z)} + W_{m(x,y,z)} V_{m(x,y,z)} \kappa'_{m(x,y,z)} + W_{w(x,y,z)} V_{w(x,y,z)} \kappa'_{w(x,y,z)} \\ & + W_{i(x,y,z)} V_{i(x,y,z)} \kappa'_{i(x,y,z)} + W_{a(x,y,z)} V_{a(x,y,z)} \kappa'_{a(x,y,z)}) / (W_{o(x,y,z)} V_{o(x,y,z)} + W_{m(x,y,z)} V_{m(x,y,z)} \\ & + W_{w(x,y,z)} V_{w(x,y,z)} + W_{i(x,y,z)} V_{i(x,y,z)} + W_{a(x,y,z)} V_{a(x,y,z)}) \end{aligned}$$

$$\kappa_{s(x,y)} = 8.28 \times 10^{-5} + 8.42 \times 10^{-4} \rho_s \quad (\rho_s < 0.156)$$

thermal conductivity of soil and surface litter

[D12d]

$$\kappa_{s(x,y)} = 4.97 \times 10^{-4} - 3.64 \times 10^{-3} \rho_s + 1.16 \times 10^{-2} \rho_s^2 \quad (\rho_s > 0.156)$$

thermal conductivity of snow

[D12e]

thermal conductivity of snow

$$G_{x(x-I,y,z)} - G_{x(x,y,z)} + G_{y(x,y-I,z)} - G_{y(x,y,z)} + G_{z(x,y,z-I)} - G_{z(x,y,z)} + LQ_{f(x,y,z)} + c_{(x,y,z)} (T_{(x,y,z)} - T'_{(x,y,z)}) / \Delta t = 0$$

3D general heat flux equation driving freezing-thawing in snowpack, surface residue and soil layers

[D13]

### Gas Flux

$Q_{dsx,y,z} = a_{gsx,y,z} D_{dy} (S'_{\gamma} f_{d,y,z} [\gamma_{gs}]_{x,y,z} - [\gamma_{ss}]_{x,y,z})$	volatilization – dissolution between aqueous and gaseous phases in soil and root	[D14a]
$Q_{dryx,y,z} = a_{grx,y,z} D_{dy} (S'_{\gamma} f_{d,y,z} [\gamma_{gr}]_{x,y,z} - [\gamma_{sr}]_{x,y,z})$		[D14b]
$Q_{gs\gamma x,y,I} = g_{ax,y} \{ [\gamma_a] - \{ 2 [\gamma_{gs}]_{x,y,I} D_{gs\gamma z(x,y,I)} / L_{z(x,y,I)} + g_{ax,y} [\gamma_a] \} / \{ 2 D_{gs\gamma z(x,y,I)} / L_{z(x,y,I)} + g_{ax,y} \} \}$	volatilization – dissolution between gaseous and aqueous phases at the soil surface ( $z = I$ ) and the atmosphere	[D15a]
$Q_{ds\gamma x,y,I} = a_{gsx,y,I} D_{dy} (S'_{\gamma} f_{d,y,I} [\gamma_a] - [\gamma_{ss}]_{x,y,I})$		[D15b]
$Q_{gs\gamma x(x,y,z)} = - Q_{wx(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma x(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x+I,y,z}) / (L_{x(x,y,z)} + L_{x(x+I,y,z)})$	3D convective - conductive gas flux among soil layers in $x$ (EW), $y$ (NS) and $z$ (vertical) directions,	[D16a]
$Q_{gs\gamma y(x,y,z)} = - Q_{wy(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma y(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y+I,z}) / (L_{y(x,y,z)} + L_{y(x,y+I,z)})$		[D16b]
$Q_{gs\gamma z(x,y,z)} = - Q_{wz(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma z(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y,z+I}) / (L_{z(x,y,z)} + L_{z(x,y,z+I)})$		[D16c]
$Q_{gr\gamma z(x,y,z)} = D_{gr\gamma z(x,y,z)} ([\gamma_{gr}]_{x,y,z} - [\gamma_a]) / \Sigma_{1,z} L_{z(x,y,z)}$	convective - conductive gas flux between roots and the atmosphere	[D16d]
$D_{gs\gamma x(x,y,z)} = D'_{g\gamma} f_{gx,y,z} [0.5 (\theta_{gx,y,z} + \theta_{gx+I,y,z})]^2 / \theta_{psx,y,z}^{0.67}$	gasous diffusivity as a function of air-filled porosity in soil	[D17a]
$D_{gs\gamma y(x,y,z)} = D'_{g\gamma} f_{gy,y,z} [0.5 (\theta_{gy,y,z} + \theta_{gy,y+I,z})]^2 / \theta_{psx,y,z}^{0.67}$		[D17b]
$D_{gs\gamma z(x,y,z)} = D'_{g\gamma} f_{gz,y,z} [0.5 (\theta_{gz,y,z} + \theta_{gz,y,z+I})]^2 / \theta_{psx,y,z}^{0.67}$		[D17c]
$D_{gr\gamma z(x,y,z)} = D'_{g\gamma} f_{gz,y,z} \theta_{prx,y,z}^{1.33} A_{r(x,y,z)} / A_{x,y}$	gasous diffusivity as a function of air-filled porosity in roots	[D17d]
$Q_{byz} = \min[0.0, \{(44.64 \theta_{wx,y,z} 273.16 / T_{x,y,z}) - \Sigma_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,y,z} M_{\gamma}))\} \\ ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,y,z} M_{\gamma})) / \Sigma_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,y,z} M_{\gamma})) S'_{\gamma} f_{d,y,z} M_{\gamma} V_{x,y,z}$	bubbling (-ve flux) when total of all partial gas pressures exceeds atmospheric pressure	[D18]

### Solute Flux

$Q_{\text{ayx}(x,y,z)} = Q_{\text{wx}(x,y,z)} [\gamma_{\text{ss}}]_{x,y,z} + 2 D_{s\gamma x(x,y,z)} ([\gamma_s]_{x,y,z} - [\gamma_s]_{x+I,y,z}) / (L_{x(x,y,z)} + L_{x(x+I,y,z)})$	3D convective - dispersive solute flux among soil layers in $x$ (EW), $y$ (NS) and $z$ (vertical) directions	[D19a]
$Q_{\text{ayy}(x,y,z)} = Q_{\text{wy}(x,y,z)} [\gamma_{\text{ss}}]_{x,y,z} + 2 D_{s\gamma y(x,y,z)} ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y+I,z}) / (L_{y(x,y,z)} + L_{y(x,y+I,z)})$		[D19b]
$Q_{\text{ayz}(x,y,z)} = Q_{\text{wz}(x,y,z)} [\gamma_{\text{ss}}]_{x,y,z} + 2 D_{s\gamma z(x,y,z)} ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y,z+I}) / (L_{z(x,y,z)} + L_{z(x,y,z+I)})$		[D19c]
$Q_{\text{ry}(x,y,z)} = Q_{\text{wr}(x,y,z)} [\gamma_{\text{ss}}]_{x,y,z} + 2\pi L_{i,r} D_{s\gamma} ([\gamma_{\text{ss}}] - [\gamma_{\text{rri},r}]) \ln\{ (r_s + r_{\text{ri},r}) / r_{\text{ri},r} \} + 2\pi L_{i,r} D_{r\gamma} ([\gamma_{\text{sti},r}] - [\gamma_{\text{rri},r}]) \ln(r_{\text{qi},r}) / r_{\text{ri},r}$	convective - dispersive solute flux between soil and root aqueous phases	[D19d]
$D_{s\gamma x(x,y,z)} = D_{\text{qx}(x,y,z)}  Q_{\text{wx}(x,y,z)}  + D'_{s\gamma} f_{\text{tx},y,z} [0.5(\theta_{\text{wx},y,z} + \theta_{\text{wx+I},y,z})] \tau$	aqueous dispersivity in soil as functions of water flux and water-filled porosity in $x$ , $y$ and $z$ directions	[D20a]
$D_{s\gamma y(x,y,z)} = D_{\text{qy}(x,y,z)}  Q_{\text{wy}(x,y,z)}  + D'_{s\gamma} f_{\text{tx},y,z} [0.5(\theta_{\text{wx},y,z} + \theta_{\text{wx+I},y,z})] \tau$		[D20b]
$D_{s\gamma z(x,y,z)} = D_{\text{qz}(x,y,z)}  Q_{\text{wz}(x,y,z)}  + D'_{s\gamma} f_{\text{tx},y,z} [0.5(\theta_{\text{wx},y,z} + \theta_{\text{wx+I},y,z})] \tau$		[D20c]
$D_{\text{ry}(x,y,z)} = D'_{\text{qr}}  Q_{\text{wr}(x,y,z)}  + D'_{s\gamma} f_{\text{tx},y,z} \theta_{\text{wx},y,z} \tau$	aqueous dispersivity to roots as functions of water flux and water-filled porosity	[D20d]
$D_{\text{qx}(x,y,z)} = 0.5 \alpha (L_{x(x,y,z)} + L_{x(x+I,y,z)})^\beta$	dispersivity as a function of water flow length	[D21a]
$D_{\text{qy}(x,y,z)} = 0.5 \alpha (L_{y(x,y,z)} + L_{y(x,y+I,z)})^\beta$		[D21b]
$D_{\text{qz}(x,y,z)} = 0.5 \alpha (L_{z(x,y,z)} + L_{z(x,y,z+I)})^\beta$		[D21c]

## Definition of Variables in Table S4

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
$x$	grid cell position in west to east direction				

$y$	grid cell position in north to south direction			
$z$	grid cell position in vertical direction		$z = 0$ : surface residue, $z = 1$ to $n$ : soil layers	
<i>variables</i>				
$A$	area of landscape position	$\text{m}^2$	[D17c]	
$A_r$	root cross-sectional area of landscape position	$\text{m}^2$	[D17c]	
$a_{gr}$	air-water interfacial area in roots	$\text{m}^2 \text{ m}^{-2}$	[D14b]	
$a_{gs}$	air-water interfacial area in soil	$\text{m}^2 \text{ m}^{-2}$	[D14a,D15b]	Skopp (1985)
$\alpha$	dependence of $D_q$ on $L$	-	[D21]	0.20
$\beta$	dependence of $D_q$ on $L$	-	[D21]	1.07
$c$	heat capacity of soil	$\text{MJ m}^{-2} \text{ }^\circ\text{C}^{-1}$	[D13]	
$c_w$	heat capacity of water	$\text{MJ m}^{-3} \text{ }^\circ\text{C}^{-1}$	[D12]	4.19
$D_{d\gamma}$	volatilization - dissolution transfer coefficient for gas $\gamma$	$\text{m}^2 \text{ h}^{-1}$	[D14,D15a]	
$D_{g\gamma}$	gaseous diffusivity of gas $\gamma$ in roots	$\text{m}^2 \text{ h}^{-1}$	[D16d,D17d]	Luxmoore et al. (1970a,b)
$D_{g\gamma}$	gaseous diffusivity of gas $\gamma$ in soil	$\text{m}^2 \text{ h}^{-1}$	[D15a,D16a,b,c,D 17a,b,c]	Millington and Quirk (1960)
$D'_{g\gamma}$	diffusivity of gas $\gamma$ in air at $0 \text{ }^\circ\text{C}$	$\text{m}^2 \text{ h}^{-1}$	[D17]	$6.43 \times 10^{-2}$ for $\gamma = \text{O}_2$
$D'_{qr}$	dispersivity in roots	$\text{m}$	[D20d]	0.004
$D_q$	dispersivity in soil	$\text{m}$	[D20,D21]	
$D_{r\gamma}$	aqueous diffusivity of gas or solute $\gamma$ in roots	$\text{m}^2 \text{ h}^{-1}$	[D19d,D20d]	

$D_{s\gamma}$	aqueous diffusivity of gas or solute $\gamma$ in soil	$\text{m}^2 \text{ h}^{-1}$	[D19,D20]	
$D'_{s\gamma}$	diffusivity of gas $\gamma$ in water at 0 °C	$\text{m}^2 \text{ h}^{-1}$	[D20]	$8.57 \times 10^{-6}$ for $\gamma = \text{O}_2$ Campbell (1985)
$d_m$	depth of mobile surface water	m	[D1a,D2,D5a,D6]	
$d_i$	depth of surface ice	m	[D2]	
$d_s$	maximum depth of surface water storage	m	[D2,D5b]	
$d_t$	depth of external water table	m	[D10]	
$d_w$	depth of surface water	m	[D1,D2]	
$d_z$	depth to mid-point of soil layer	m	[D10]	
$E$	evaporation or transpiration flux	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D4,D11]	
$e_a$	atmospheric vapor density	$\text{m}^3 \text{ m}^{-3}$	[D6]	
$e_{l(T_l, \psi_l)}$	surface litter vapor density at current $T_l$ and $\psi_l$	$\text{g m}^{-3}$	[D6a]	
$e_{s(T_s, \psi_s)}$	soil surface vapor density at current $T_s$ and $\psi_s$	$\text{g m}^{-3}$	[D6b]	
$F$	rate constant for lateral transfer of $V_{(s,w,i)}$	$\text{h}^{-1}$	[D1b]	0.005
$f_{d\gamma}$	temperature dependence of $D'_{s\gamma}$	-	[D14,D15b,D18]	Wilhelm et al. (1977)
$f_{t_g}$	temperature dependence of $D'_{g\gamma}$	-	[D17]	Campbell (1985)
$f_{t_s}$	temperature dependence of $D'_{s\gamma}$	-	[D20]	Campbell (1985)
$G$	soil surface heat flux	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D11]	
$G_x, G_y, G_z$	soil heat flux in $x, y$ or $z$ directions	$\text{MJ m}^{-2} \text{ h}^{-1}$	[D12,D13]	
$g_a$	boundary layer conductance	$\text{m h}^{-1}$	[D15a]	

$\gamma$	gas ( $\text{H}_2\text{O}$ , $\text{CO}_2$ , $\text{O}_2$ , $\text{CH}_4$ , $\text{NH}_3$ , $\text{N}_2\text{O}$ , $\text{N}_2$ , $\text{H}_2$ ) or solute (from S5)		[D14,D15]
$[\gamma_a]$	atmospheric concentration of gas $\gamma$	$\text{g m}^{-3}$	[D15,D16d]
$[\gamma_{gr}]$	gasous concentration of gas $\gamma$ in roots	$\text{g m}^{-3}$	[D14b,D16d]
$[\gamma_{gs}]$	gasous concentration of gas $\gamma$ in soil	$\text{g m}^{-3}$	[D14a,D15a,D16a, D16b,D16c]
$[\gamma_{sr}]$	aqueous concentration of gas $\gamma$ in roots	$\text{g m}^{-3}$	[D14b, D19d]
$[\gamma_{rr}]$	aqueous concentration of gas $\gamma$ at root surface	$\text{g m}^{-3}$	[D19b]
$[\gamma_{ss}]$	aqueous concentration of gas $\gamma$ in soil	$\text{g m}^{-3}$	[D14a,D15b,D18, D19]
$H$	sensible heat flux	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11]
$K$	hydraulic conductivity	$\text{m}^2 \text{MPa}^{-1} \text{h}^{-1}$	[D9,D10] Green and Corey (1971)
$K'_x, K'_y, K'_z$	hydraulic conductance in $x$ , $y$ or $z$ directions	$\text{m MPa}^{-1} \text{h}^{-1}$	[D7,D9]
$\kappa$	bulk thermal conductivity of soil or surface litter	$\text{MJ m}^{-1} \text{h}^{-1} \text{^oC}^{-1}$	[D12a,b,c,d,e] de Vries (1963)
$\kappa_s$	bulk thermal conductivity of snowpack	$\text{MJ m}^{-1} \text{h}^{-1} \text{^oC}^{-1}$	[D12e] Sturm et al. (1997)
$\kappa'_{0, m, w, i, a}$	thermal conductivity of organic matter, mineral water, ice and air	$\text{MJ m}^{-1} \text{h}^{-1} \text{^oC}^{-1}$	[D12d] $9.05 \times 10^{-4}, 1.06 \times 10^{-2}, 2.07 \times 10^{-3}, 7.84 \times 10^{-3}, 9.05 \times 10^{-5}$
$L_i$	root length	$\text{m m}^{-2}$	[D19d]
$L_t$	distance from boundary to external water table in $x$ or $y$ directions	$\text{m}$	[D10]
$L_x, L_y, L_z$	length of landscape element in $x$ , $y$ or $z$ directions	$\text{m}$	[D1a,D1b,D5b,D8, D9,D10,D12,D15 a,D16,D19]
$LE_l$	latent heat flux from surface litter	[D6a] $\text{MJ m}^{-2} \text{h}^{-1}$	

$LE_s$	latent heat flux from soil surface	$[D6b]$	$\text{MJ m}^{-2} \text{ h}^{-1}$
$L$	latent heat of evaporation	$\text{MJ m}^{-3}$	[D6,D11,D13] 2460
$M_\gamma$	atomic mass of gas $\gamma$	$\text{g mol}^{-1}$	[D18]
$P$	precipitation flux	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D4]
$Q_{\text{ay}}$	aqueous flux of gas or solute $\gamma$ in soil	$\text{g m}^{-2} \text{ h}^{-1}$	[D19a,b,c]
$Q_{\text{byz}}$	bubbling flux	$\text{g m}^{-2} \text{ h}^{-1}$	[D18]
$Q_{\text{dry}}$	volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in roots	$\text{g m}^{-2} \text{ h}^{-1}$	[D14b]
$Q_{\text{ds}\gamma}$	volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in soil	$\text{g m}^{-2} \text{ h}^{-1}$	[D14a,D15b]
$Q_f$	freeze-thaw flux (thaw +ve)	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D8,D13]
$Q_{\text{gr}\gamma}$	gaseous flux of gas $\gamma$ between roots and the atmosphere	$\text{g m}^{-2} \text{ h}^{-1}$	[D16d]
$Q_{\text{gs}\gamma}$	gaseous flux of gas $\gamma$ in soil	$\text{g m}^{-2} \text{ h}^{-1}$	[D15a,D16a,b,c]
$Q_{\text{rx}}, Q_{\text{ry}}$	surface water flow in $x$ or $y$ directions	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D1a,D4]
$Q_{\text{ry}}$	aqueous flux of gas or solute $\gamma$ from soil and root aqueous phases to root surface	$\text{g m}^{-2} \text{ h}^{-1}$	[D19d]
$Q_{(\text{s},\text{w},\text{i})}$	lateral redistribution of snowpack snow $s$ , water $w$ and ice $i$ in $x$ or $y$ directions	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D1b]
$Q_t$	water flux between boundary grid cell and external water table in $x$ or $y$ directions	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D10]
$Q_{\text{wr}}$	root water uptake	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D19d, D20d]
$Q_{\text{w},\text{x}}, Q_{\text{w},\text{y}}, Q_{\text{w},\text{z}}$	subsurface water flow in $x$ , $y$ or $z$ directions	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[D4,D7,D8,D12,D16,D19,D20]
$\theta_{FC}$	water content at field capacity	$\text{m}^3 \text{ m}^{-3}$	[D7d]

$\theta_g$	air-filled porosity	$\text{m}^3 \text{ m}^{-3}$	[D17a,b,c]		
$\theta_{\text{pr}}$	root porosity	$\text{m}^3 \text{ m}^{-3}$	[D17d]	dryland spp. 0.10 wetland spp. 0.20	Luxmoore et al. (1970a,b)
$\theta_{\text{ps}}$	soil porosity	$\text{m}^3 \text{ m}^{-3}$	[D17a,b,c]		
$\theta_{\text{ST}}$	water content at saturation	$\text{m}^3 \text{ m}^{-3}$	[D7d]		from BD
$\theta_w$	water-filled porosity	$\text{m}^3 \text{ m}^{-3}$	[D8,D18,D20]		
$\theta_{\text{WP}}$	water content at wilting point	$\text{m}^3 \text{ m}^{-3}$	[D7d]		
$R$	ratio of cross-sectional area to perimeter of surface flow	$\text{m}$	[D3,D5a]		
$R_n$	net radiation	$\text{MJ m}^{-2} \text{ h}^{-1}$	[D11]		
$r_{\text{al}}$	surface litter boundary layer resistance	$\text{m h}^{-1}$	[D6a]		
$r_{\text{as}}$	Soil surface boundary layer resistance	$\text{m h}^{-1}$	[D6b]		
$r_{\text{qi},r}$	radius of root or mycorrhizal aerenchyma	$\text{m}$	[D19d]		
$r_{\text{ri},r}$	root or mycorrhizal radius	$\text{m}$	[D19d]	$1.0 \times 10^{-4}$ or $5.0 \times 10^{-6}$	
$r_s$	thickness of soil water films	$\text{m}$	[D19d, D21d]		
$\rho_s$	density of snowpack	$\text{Mg m}^{-3}$	[D12e]		
$S'_{\gamma}$	Ostwald solubility coefficient of gas $\gamma$ at 30 °C	-	[D14,D15b,D18]	0.0293 for $\gamma = \text{O}_2$	Wilhelm et al. (1977)
$s_r$	slope of channel sides during surface flow	$\text{m m}^{-1}$	[D5a]		
$s_x, s_y$	slope in $x$ or $y$ directions	$\text{m m}^{-1}$	[D3,D5b]		
$T$	soil temperature	°C	[D12,D18]		

$\tau$	tortuosity	-	[D20]	
$V_{o, m, w, i, a}$	volumetric ratios of organic matter, mineral water, ice and air	-	[D12d]	
$V_{(s,w,i)}$	Volume of snow $s$ , water $w$ and ice $i$ in snowpack	$\text{m}^3 \text{ m}^{-2}$	[D1b]	
$v_x, v_y$	velocity of surface flow in $x$ or $y$ directions	$\text{m h}^{-1}$	[D1a,D3]	
$W_{o, m, w, i, a}$	weighting factors for organic matter, mineral water, ice and air	-	[D12d]	1.253, 0.514, 1.00 de Vries (1963) 0.611, 1.609
$\psi_s$	soil water potential at saturation	MPa	[D10]	$5.0 \times 10^{-3}$
$\psi_{mg}$	soil gravimetric potential	MPa	[D7e]	-0.03
$\psi_{FC}$	soil matric potential at field capacity	MPa	[D7d]	
$\psi_m$	soil matric potential	MPa	[D7d,e]	-1.5
$\psi_{WP}$	soil matric potential at wilting point	MPa	[D7d,e]	
$\psi_\pi$	soil osmotic potential	MPa	[D7e]	
$\psi_s$	soil water potential	MPa	[D7,D10]	
$Z$	surface elevation	m	[D1b,D5b]	
$z_s$	snowpack depth	m	[D1b]	
$z_r$	Manning's roughness coefficient	$\text{m}^{-1/3} \text{ h}$	[D3]	0.01

## **S5: Solute Transformations**

### *Precipitation - Dissolution Equilibria*

Solution  $[\text{NH}_4^+]$ ,  $[\text{NO}_3^-]$  and  $[\text{H}_2\text{PO}_4^-]$  that drive  $U_{\text{NH}_4}$ ,  $U_{\text{NO}_3}$  and  $U_{\text{PO}_4}$  [C23] are controlled by precipitation, adsorption and ion pairing reactions (Grant et al., 2004; Grant and Heaney, 1997), including precipitation-dissolution of  $\text{Al}(\text{OH})_3$ ,  $\text{Fe}(\text{OH})_3$ ,  $\text{CaCO}_3$ ,  $\text{CaSO}_4$ ,  $\text{AlPO}_4$ ,  $\text{FePO}_4$ ,  $\text{Ca}(\text{H}_2\text{PO}_4)_2$ ,  $\text{CaHPO}_4$ , and  $\text{Ca}_5(\text{PO}_4)_3\text{OH}$  [E1 – E9], cation exchange between  $\text{Ca}^{2+}$ ,  $\text{NH}_4^+$  and other cations [E10 – E15], anion exchange between adsorbed and soluble  $\text{H}_2\text{PO}_4^-$ ,  $\text{HPO}_4^{2-}$  and  $\text{OH}^-$  [E16 – E20], and ion pairing [E22 – E55].

**Table S5: Solute Transformations**

<i>Precipitation - Dissolution Equilibria</i>			
$\text{Al(OH)}_{3(s)} \rightleftharpoons (\text{Al}^{3+}) + 3 (\text{OH}^-)$	(amorphous $\text{Al(OH)}_3$ )	-33.0	[E1] <sup>1</sup>
$\text{Fe(OH)}_{3(s)} \rightleftharpoons (\text{Fe}^{3+}) + 3 (\text{OH}^-)$	(soil Fe)	-39.3	[E2]
$\text{CaCO}_{3(s)} \rightleftharpoons (\text{Ca}^{2+}) + (\text{CO}_3^{2-})$	(calcite)	-9.28	[E3]
$\text{CaSO}_{4(s)} \rightleftharpoons (\text{Ca}^{2+}) + (\text{SO}_4^{2-})$	(gypsum)	-4.64	[E4]
$\text{AlPO}_{4(s)} \rightleftharpoons (\text{Al}^{3+}) + (\text{PO}_4^{3-})$	(variscite)	-22.1	[E5] <sup>2</sup>
$\text{FePO}_{4(s)} \rightleftharpoons (\text{Fe}^{3+}) + (\text{PO}_4^{3-})$	(strengeite)	-26.4	[E6]
$\text{Ca}(\text{H}_2\text{PO}_4)_{2(s)} \rightleftharpoons (\text{Ca}^{2+}) + 2 (\text{H}_2\text{PO}_4^-)$	(monocalcium phosphate)	-1.15	[E7] <sup>3</sup>
$\text{CaHPO}_{4(s)} \rightleftharpoons (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	(monetite)	-6.92	[E8]
$\text{Ca}_5(\text{PO}_4)_3\text{OH}_{(s)} \rightleftharpoons 5 (\text{Ca}^{2+}) + 3 (\text{PO}_4^{3-}) + (\text{OH}^-)$	(hydroxyapatite)	-58.2	[E9]
<i>Cation Exchange Equilibria</i> <sup>4</sup>			
$\text{X-Ca} + 2 (\text{NH}_4^+) \rightleftharpoons 2 \text{X-NH}_4 + (\text{Ca}^{2+})$		1.00	[E10]
$3 \text{X-Ca} + 2 (\text{Al}^{3+}) \rightleftharpoons 2 \text{X-Al} + 3 (\text{Ca}^{2+})$		1.00	[E11]
$\text{X-Ca} + (\text{Mg}^+) \rightleftharpoons \text{X-Mg} + (\text{Ca}^{2+})$		0.60	[E12]
$\text{X-Ca} + 2 (\text{Na}^+) \rightleftharpoons 2 \text{X-Na} + (\text{Ca}^{2+})$		0.16	[E13]
$\text{X-Ca} + 2 (\text{K}^+) \rightleftharpoons 2 \text{X-K} + (\text{Ca}^{2+})$		3.00	[E14]
$\text{X-Ca} + 2 (\text{H}^+) \rightleftharpoons 2 \text{X-H} + (\text{Ca}^{2+})$		1.00	[E15]
$3 \text{X-Al} + 2 (\text{X-Ca} + \text{X-Mg}) + \text{X-NH}_4 + \text{X-K} + \text{X-Na} + \text{X-H} = \text{CEC}$			[E16]

<sup>1</sup> Round brackets denote solute activity. Numbers in italics denote  $\log K$  (precipitation-dissolution, ion pairs), Gapon coefficient (cation exchange) or  $\log c$  (anion exchange).

<sup>2</sup> All equilibrium reactions involving N and P are calculated for both band and non-band volumes if a banded fertilizer application has been made. These volumes are calculated dynamically from diffusive transport of soluble N and P.

<sup>3</sup> May only be entered as fertilizer, not considered to be naturally present in soils.

<sup>4</sup> X- denotes surface exchange site for cation or anion adsorption.

*Anion Adsorption Equilibria*

$\text{X-OH}_2^+ \Leftrightarrow \text{X-OH} + (\text{H}^+)$	-7.35	[E17]
$\text{X-OH} \Leftrightarrow \text{X-O}^- + (\text{H}^+)$	-8.95	[E18]
$\text{X-H}_2\text{PO}_4^- + \text{H}_2\text{O} \Leftrightarrow \text{X-OH}_2^+ + (\text{H}_2\text{PO}_4^{2-})$	-2.80	[E19]
$\text{X-H}_2\text{PO}_4^- + (\text{OH}^-) \Leftrightarrow \text{X-OH} + (\text{H}_2\text{PO}_4^{2-})$	4.20	[E20]
$\text{X-HPO}_4^{2-} + (\text{OH}^-) \Leftrightarrow \text{X-OH} + (\text{HPO}_4^{2-})$	2.60	[E21]
$\text{X-OH}_2^+ + \text{X-OH} + \text{X-O}^- + \text{X-H}_2\text{PO}_4^- + \text{X-HPO}_4^{2-} + \text{X-COO}^- = \text{AEC}$		[E22]

*Organic Acid Equilibria*

$\text{X-COOH} \Leftrightarrow \text{X-COO}^- + (\text{H}^+)$	-5.00	[E23]
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*Ion Pair Equilibria*

$(\text{NH}_4^+) \Leftrightarrow (\text{NH}_3)_{(\text{s})} + (\text{H}^+)$	-9.24	[E24]
$\text{H}_2\text{O} \Leftrightarrow (\text{H}^+) + (\text{OH}^-)$	-14.3	[E25]
$(\text{CO}_2)_{(\text{g})} + \text{H}_2\text{O} \Leftrightarrow (\text{H}^+) + (\text{HCO}_3^-)$	-6.42	[E26]
$(\text{HCO}_3^-) \Leftrightarrow (\text{H}^+) + (\text{CO}_3^{2-})$	-10.4	[E27]
$(\text{AlOH})_{2+} \Leftrightarrow (\text{Al}^{3+}) + (\text{OH}^-)$	-9.06	[E28]
$(\text{Al}(\text{OH})_2^+) \Leftrightarrow (\text{AlOH})_{2+} + (\text{OH}^-)$	-10.7	[E29]
$(\text{Al}(\text{OH})_3^0) \Leftrightarrow (\text{Al}(\text{OH})_2^+) + (\text{OH}^-)$	-5.70	[E30]
$(\text{Al}(\text{OH})_4^-) \Leftrightarrow (\text{Al}(\text{OH})_3^0) + (\text{OH}^-)$	-5.10	[E31]
$(\text{AlSO}_4^+) \Leftrightarrow (\text{Al}^{3+}) + (\text{SO}_4^{2-})$	-3.80	[E32]
$(\text{FeOH})_{2+} \Leftrightarrow (\text{Fe}^{3+}) + (\text{OH}^-)$	-12.1	[E33]
$(\text{Fe}(\text{OH})_2^+) \Leftrightarrow (\text{FeOH})_{2+} + (\text{OH}^-)$	-10.8	[E34]
$(\text{Fe}(\text{OH})_3^0) \Leftrightarrow (\text{Fe}(\text{OH})_2^+) + (\text{OH}^-)$	-6.94	[E35]
$(\text{Fe}(\text{OH})_4^-) \Leftrightarrow (\text{Fe}(\text{OH})_3^0) + (\text{OH}^-)$	-5.84	[E36]

$(\text{FeSO}_4^{+}) \Leftrightarrow (\text{Fe}^{3+}) + (\text{SO}_4^{2-})$	-4.15	[E37]
$(\text{CaOH}_0^{+}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{OH}^{-})$	-1.90	[E38]
$(\text{CaCO}_3^{0}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{CO}_3^{2-})$	-4.38	[E39]
$(\text{CaHCO}_3^{0}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{HCO}_3^{-})$	-1.87	[E40]
$(\text{CaSO}_4^{0}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{SO}_4^{2-})$	-2.92	[E41]
$(\text{MgOH}_0^{+}) \Leftrightarrow (\text{Mg}^{2+}) + (\text{OH}^{-})$	-3.15	[E42]
$(\text{MgCO}_3^{0}) \Leftrightarrow (\text{Mg}^{2+}) + (\text{CO}_3^{2-})$	-3.52	[E43]
$(\text{MgHCO}_3^{0}) \Leftrightarrow (\text{Mg}^{2+}) + (\text{HCO}_3^{-})$	-1.17	[E44]
$(\text{MgSO}_4^{0}) \Leftrightarrow (\text{Mg}^{2+}) + (\text{SO}_4^{2-})$	-2.68	[E45]
$(\text{NaCO}_3^{-}) \Leftrightarrow (\text{Na}^{+}) + (\text{CO}_3^{2-})$	-3.35	[E46]
$(\text{NaSO}_4^{-}) \Leftrightarrow (\text{Na}^{+}) + (\text{SO}_4^{2-})$	-0.48	[E47]
$(\text{KSO}_4^{-}) \Leftrightarrow (\text{K}^{+}) + (\text{SO}_4^{2-})$	-1.30	[E48]
$(\text{H}_3\text{PO}_4) \Leftrightarrow (\text{H}^{+}) + (\text{H}_2\text{PO}_4^{-})$	-2.15	[E49]
$(\text{H}_2\text{PO}_4^{2-}) \Leftrightarrow (\text{H}^{+}) + (\text{HPO}_4^{2-})$	-7.20	[E50]
$(\text{HPO}_4^{2-}) \Leftrightarrow (\text{H}^{+}) + (\text{PO}_4^{3-})$	-12.4	[E51]
$(\text{FeH}_2\text{PO}_4^{2+}) \Leftrightarrow (\text{Fe}^{3+}) + (\text{H}_2\text{PO}_4^{-})$	-5.43	[E52]
$(\text{FeHPO}_4^{+}) \Leftrightarrow (\text{Fe}^{3+}) + (\text{HPO}_4^{2-})$	-10.9	[E53]
$(\text{CaH}_2\text{PO}_4^{0}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{H}_2\text{PO}_4^{-})$	-1.40	[E54]
$(\text{CaHPO}_4^{0}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	-2.74	[E55]
$(\text{CaPO}_4^{-}) \Leftrightarrow (\text{Ca}^{2+}) + (\text{PO}_4^{3-})$	-6.46	[E56]
$(\text{MgHPO}_4^{0}) \Leftrightarrow (\text{Mg}^{2+}) + (\text{HPO}_4^{2-})$	-2.91	[E57]

## **S6: N<sub>2</sub> Fixation**

### *Microbial Growth*

Modelling the activity of symbiotic N<sub>2</sub> fixing bacteria in roots (e.g. *Rhizobia*) and branches (e.g. cyanobacteria) follows a protocol similar to that of non-symbiotic N<sub>2</sub> fixing bacteria in soil. Respiration demand is driven by specific activity, microbial biomass  $M_n$ , and nonstructural C concentration [ $\chi_n$ ] in root or branch nodules [F1], and is constrained by temperature [F2] and microbial N or P status [F3]. Nodule respiration  $R$  in roots is constrained by the extent to which O<sub>2</sub> uptake meets O<sub>2</sub> demand [F4] imposed by respiration demand [F5]. O<sub>2</sub> uptake is in turn constrained by rhizosphere [O<sub>2r</sub>] [F6a] which is controlled by radial diffusion of O<sub>2</sub> through soil water to roots and nodules [F6b]. Soil water [O<sub>2</sub>] is maintained by dissolution of O<sub>2</sub> from soil air which is in turn maintained by soil-atmosphere gas exchange and vertical diffusion (Grant, 2004).  $R_h$  is first allocated to maintenance respiration  $R_m$  [F7 – F8] and the remainder if any is allocated to growth respiration  $R_g$  [F9]. If  $R_m$  exceeds  $R_h$ , the shortfall is made up from respiration of microbial protein C, forcing senescence and litterfall of associated non-protein C [F10 – F11].

### *N<sub>2</sub> Fixation*

N<sub>2</sub> fixation  $V_{N_2}$  is driven by  $R_g$  [F12], but is constrained by accumulation of nonstructural N  $\nu_n$  with respect to nonstructural C and P also required for microbial growth in the root or branch nodule [F13]. Nonstructural N  $\nu_{nd}$  is the product of  $V_{N_2}$ , so that [F12] simulates the inhibition of N<sub>2</sub> fixation by its product (Postgate, 1998). The value of  $V_{N_2}$  is also limited by the additional N needed to maintain bacterial N content [ $N_n'$ ] of  $M_n$  [F12] (typically 1/8 that of C), so that N<sub>2</sub> fixation is constrained by the need of nodule bacteria for N not met from other sources (Postgate, 1998). Respiration required for N<sub>2</sub> fixation  $R_{N_2}$  [F14] is subtracted from  $R_g$  [F15] when calculating microbial growth [F16 – F18]. Microbial senescence drives N and P litterfall [F19 – F20].

### *Nodule – Root Exchange*

Exchange of nonstructural C, N and P between roots or branches and nodules is driven by concentration gradients [F21 – F23] created by generation, transfer and consumption of nonstructural C, N and P in shoots, roots, mycorrhizae and nodules. Nonstructural C is generated in branches and transferred along concentration gradients to roots and thence to nodules [F21]. Nonstructural P is generated in roots and transferred along concentration gradients to branches and nodules [F23]. Nonstructural N is generated in roots through mineral uptake and in nodules through gaseous fixation [F22]. Nonstructural C, N and P in nodules is determined by root-nodule and branch-nodule exchange, by nodule respiration and fixation, and by remobilization from nodule litterfall [F24 – F26].

Root nonstructural N ( $\nu_r$ ) may rise if high mineral N concentrations in soil sustain rapid N uptake by roots. Large  $\nu_r$  suppresses or even reverses the transfer of  $\nu_n$  from nodule to root or branch [F22], raising  $\nu_n$  [F25] and hence suppressing  $V_{N_2}$  [F12 – F13]. Large  $\nu_r$  also accelerates the consumption of  $\chi_r$ , slowing its transfer to nodules [F21], reducing  $\chi_n$  [F24] and hence slowing nodule growth [F1]. Conversely, slow root N uptake caused by low soil mineral N concentrations would lower  $\nu_{rt}$  and raise  $\chi_{rt}$ , hastening the transfer of  $\nu_n$  from nodule to root or branch and of  $\chi_{rt}$  from root or branch to nodule, lowering  $\nu_n$ , raising  $\chi_n$ , and accelerating  $V_{N_2}$ . However [F13] also allows  $V_{N_2}$  to be constrained by nonstructural C and P concentrations arising from branch CO<sub>2</sub> fixation and root P uptake. All equations in S6 are solved for nodules in roots ( $i,l$ ) and branches ( $i,j$ ) except for [F6], although only those for roots are given.

**Table S6: Symbiotic N<sub>2</sub> Fixation**

<i>Microbial Growth</i>	
$R_{\max i,l} = M_{ni,l} R' [\chi_{ni,l}] / ([\chi_{ni,l}] + K_{\chi n}) f_t f_{NP}$	respiration demand [F1]
$f_t = T_l \{ \exp[B - H_a / (R T_l)] \} / \{ 1 + \exp[(H_{dl} - ST_l) / (RT_l)] + \exp[(ST_l - H_{dh}) / (R T_l)] \}$	Arrhenius function [F2]
$f_{NP} = \min\{[N_{ni,l}] / [N_n'], [P_{ni,l}] / [P_n']\}$	N or P limitation [F3]
$R_{i,l} = R_{\max i,l} (V_{O_2 i,l} / V_{O_2 \max i,l})$	O <sub>2</sub> limitation [F4]
$V_{O_2 \max i,l} = 2.67 R_{\max i,l}$	O <sub>2</sub> demand [F5]
$V_{O_2 i,l} = V_{O_2 \max i,l} [O_{2ri,l}] / ([O_{2ri,l}] + K_{O_2 r})$	equilibrate O <sub>2</sub> uptake with supply [F6a]
$= 2\pi L_{ri,l} D_{sO_2} ([O_{2l}] - [O_{2ri,l}]) / \ln((r_{ri,l} + r_{wl}) / r_{ri,l})$	[F6b]
$R_{mi,l} = R_m N_{ni,l} f_{tm}$	maintenance respiration [F7]
$f_{tm} = e^{[y(T_l - 298.16)]}$	temperature function [F8]
$R_{gi,l} = \max\{0.0, R_{i,l} - R_{mi,l}\}$	growth + fixation respiration [F9]
$R_{si,l} = \max\{0.0, R_{mi,l} - R_{i,l}\}$	microbial senescence [F10]
$L_{Ci,l} = R_{si,l} \min\{M_{ni,l} / (2.5 N_{ni,l}), M_{ni,l} / (25.0 P_{ni,l})\}$	microbial C litterfall [F11]
<i>N<sub>2</sub> Fixation</i>	
$V_{N_2 i,l} = \min\{R_{gi,l} E_{N_2}' f_{CP}, M_{ni,l} [N_n'] - N_{ni,l}\} [N_{2ri,l}] / ([N_{2ri,l}] + K_{N_2 r})$	rate of N <sub>2</sub> fixation [F12]
$f_{CP} = \min\{[\chi_{ni,l}] / (1.0 + [\nu_{ni,l}] / K_{\nu_{\chi n}}), [\pi_{ni,l}] / (1.0 + [\nu_{ni,l}] / K_{\nu \pi_n})\}$	product inhibition of N <sub>2</sub> fixation [F13]
$R_{N_2 i,l} = V_{N_2 i,l} / E_{N_2}'$	fixation respiration [F14]

$U_{\chi i,l} = (R_{gi,l} - R_{N2i,l}) / (1 - Y_n')$	growth respiration	[F15]
$\delta M_{ni,l} / \delta t = U_{i,l} Y_n' - L_{Ci,l}$	microbial C growth	[F16]
$\delta N_{ni,l} / \delta t = \delta M_{ni,l} / \delta t \min\{v_{ni,l}/\chi_{ni,l}, [N_n']\}$	microbial N growth	$\delta M_{ndi,l} / \delta t > 0$ [F17a]
$\delta N_{ni,l} / \delta t = N_{ni,l} / M_{ni,l} \delta M_{ni,l} / \delta t$	microbial N growth	$\delta M_{ndi,l} / \delta t < 0$ [F17b]
$\delta P_{ni,l} / \delta t = \delta M_{ni,l} / \delta t \min\{\pi_{ni,l}/\chi_{ni,l}, [P_n']\}$	microbial P growth	$\delta M_{ndi,l} / \delta t > 0$ [F18a]
$\delta P_{ni,l} / \delta t = P_{ni,l} / M_{ni,l} \delta M_{ni,l} / \delta t$	microbial P growth	$\delta M_{ndi,l} / \delta t < 0$ [F18b]
$L_{Ni,l} = \text{abs}(\delta N_{ni,l} / \delta t)$	microbial N litterfall	$\delta N_{ndi,l} / \delta t < 0$ [F19]
$L_{Pi,l} = \text{abs}(\delta P_{ni,l} / \delta t)$	microbial P litterfall	$\delta P_{ndi,l} / \delta t < 0$ [F20]

#### Nodule – Root Exchange

$V_{\chi i,l} = \kappa (\chi_{ri,l} M_{ni,l} - \chi_{ni,l} M_{ri,l}) / (M_{ni,l} + M_{ri,l})$	nodule–root C exchange	[F21]
$V_{vi,l} = \kappa (v_{ri,l} \chi_{ni,l} - v_{ni,l} \chi_{ri,l}) / (\chi_{ni,l} + \chi_{ri,l})$	nodule–root N exchange	[F22]
$V_{\pi i,l} = \kappa (\pi_{ri,l} \chi_{ni,l} - \pi_{ni,l} \chi_{ri,l}) / (\chi_{ni,l} + \chi_{ri,l})$	nodule–root P exchange	[F23]
$\delta \chi_{ni,l} / \delta t = V_{\chi i,l} - \min\{R_{mi,l}, R_{i,l}\} - R_{N2i,l} - U_{\chi i,l} + F_{LC,l} L_{Ci,l}$	nodule nonstructural C	[F24]
$\delta v_{ni,l} / \delta t = V_{vi,l} - \delta N_{ni,l} / \delta t + V_{N2i,l} + F_{LN,l} L_{Ni,l}$	nodule nonstructural N	[F25]
$\delta \pi_{ni,l} / \delta t = V_{\pi i,l} - \delta P_{ni,l} / \delta t + F_{LP,l} L_{Pi,l}$	nodule nonstructural P	[F26]

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#### Definition of Variables in Table S6

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Variable	Definition	Units	Equations	Input Values	Reference
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$B$	parameter such that $f_t = 1.0$ at $T_l = 298.15$ K		F2	17.533	
$\chi_{ni,l}$	nodule nonstructural C	$\text{g m}^{-2}$	F17a,F18a,F21,F22,B23,B24		
$[\chi_{ni,l}]$	nodule nonstructural C concentration	$\text{g g}^{-1}$	F1,F13		
$\chi_{ri,l}$	root nonstructural C	$\text{g m}^{-2}$	F21,F22,F23		
$D_{sO_2}$	diffusivity of aqueous $O_2$	$\text{m}^2 \text{h}^{-1}$	F6b		
$E_{N_2}'$	direct energy cost of $N_2$ fixation	$\text{g N g C}^{-1}$	F12,F14	0.25	Gutschick, (1981), Voisin et al., (2003)
$F_{LC,l}$	fraction of nodule C litterfall remobilized as nonstructural C	-	F24		
$F_{LN,l}$	fraction of nodule N litterfall remobilized as nonstructural N	-	F25		
$F_{LP,l}$	fraction of nodule P litterfall remobilized as nonstructural P	-	F26		
$f_{CP}$	effect of nodule nonstructural C or P content on $N_2$ fixation	-	F12,F13		
$f_{NP}$	effect of nodule N or P content on respiration	-	F1,F3		
$f_t$	temperature function for nodule respiration	-	F1,F2		
$f_{tm}$	temperature function for nodule maintenance respiration	-	F7,F8		
$H_a$	energy of activation	$\text{J mol}^{-1}$	F2	$57.5 \times 10^3$	
$H_{dh}$	energy of high temperature deactivation	$\text{J mol}^{-1}$	F2	$220 \times 10^3$	
$H_{dl}$	energy of low temperature deactivation	$\text{J mol}^{-1}$	F2	$190 \times 10^3$	
$K_{\chi n}$	Michaelis-Menten constant for nodule respiration of $\chi_{ndi,l}$	$\text{g g}^{-1}$	F1	0.01	
$K_{l\chi n}$	inhibition constant for nonstructural N:C on $N_2$ fixation	$\text{g g}^{-1}$	F13	10	

$K_{I\pi_n}$	inhibition constant for nonstructural N:P on N <sub>2</sub> fixation	g g <sup>-1</sup>	F13	1000
$K_{N_2r}$	Michaelis-Menten constant for nodule N <sub>2</sub> uptake	g N m <sup>-3</sup>	F12	0.14
$K_{O_2r}$	Michaelis-Menten constant for nodule O <sub>2</sub> uptake	g O m <sup>-3</sup>	F6a	0.32
$\kappa$	rate constant for nonstructural C,N,P exchange between root and nodule	h <sup>-1</sup>	F21,F22,F23	
$L_{ri,l}$	root length	m m <sup>-2</sup>	F6b	
$L_{Ci,l}$	nodule C litterfall	g C m <sup>-2</sup> h <sup>-1</sup>	F11,F16,F24	
$L_{Ni,l}$	nodule N litterfall	g N m <sup>-2</sup> h <sup>-1</sup>	F19,F25	
$L_{Pi,l}$	nodule P litterfall	g P m <sup>-2</sup> h <sup>-1</sup>	F20,F26	
$M_{ni,l}$	nodule structural C	g C m <sup>-2</sup>	F1,F11,F12,F16 ,F17,F18,F21	
$M_{ri,l}$	root structural C	g C m <sup>-2</sup>	F21	
[ $N_n'$ ]	maximum nodule structural N concentration	g N g C <sup>-1</sup>	F3,F12	0.1
$N_{ni,l}$	nodule structural N	g N m <sup>-2</sup>	F7,F11,F12,F17,F19,F25	
[ $N_{ni,l}$ ]	nodule structural N concentration	g N g C <sup>-1</sup>	F3,F17a	
[ $N_{2ri,l}$ ]	rhizosphere aqueous N <sub>2</sub> concentration	g N m <sup>-3</sup>	F12	
$v_{ni,l}$	nodule nonstructural N	g N m <sup>-2</sup>	F17a,F22,F25	
$v_{ri,l}$	root nonstructural N	g N m <sup>-2</sup>	F22	
[ $v_{ni,l}$ ]	nodule concentration of nonstructural N	g g <sup>-1</sup>	F13,F17a	
[ $O_{2ri,l}$ ]	rhizosphere aqueous O <sub>2</sub> concentration	g O m <sup>-3</sup>	F6a,b	

$[O_2]$	soil aqueous $O_2$ concentration	$g O m^{-3}$	F6b	
$[P_{n'}]$	maximum nodule structural P concentration	$g P g C^{-1}$	F3,F18a	0.01
$P_{ni,l}$	nodule structural P	$g P m^{-2}$	F18a,F20,F26	
$[P_{ni,l}]$	nodule structural P concentration	$g P g C^{-1}$	F3,F11	
$\pi_{ni,l}$	nodule nonstructural P	$g P m^{-2}$	F18a,F23,F26	
$\pi_{ri,l}$	root nonstructural P	$g P m^{-2}$	F23	
$[\pi_{ni,l}]$	nodule concentration of nonstructural P	$g g^{-1}$	F13	
$R$	gas constant	$J mol^{-1} K^{-1}$	F2	8.3143
$R_{gi,l}$	nodule growth respiration	$g C m^{-2} h^{-1}$	F9,F12,F15	
$R'$	specific nodule respiration at 25°C, and non-limiting $O_2$ , $\chi_{ndi,l}$ , $V_{ndi,l}$ and $\pi_{ndi,l}$	$h^{-1}$	F1	0.125
$R_{i,l}$	nodule respiration under ambient $O_2$	$g C m^{-2} h^{-1}$	F4,F9,F10,F24	
$R_m$	specific nodule maintenance respiration at 25°C	$g C g C^{-1} h^{-1}$	F7	
$R_{maxi,l}$	nodule respiration under non-limiting $O_2$	$g C m^{-2} h^{-1}$	F1,F4,F5	
$R_{mi,l}$	nodule maintenance respiration	$g C m^{-2} h^{-1}$	F7,F9,F10,F24	
$R_{N2i,l}$	nodule respiration for $N_2$ fixation	$g C m^{-2} h^{-1}$	F14,F15,F24	
$R_{si,l}$	nodule senescence respiration	$g C m^{-2} h^{-1}$	F9,F11	
$r_{ri,l}$	root radius	m	F6b	
$r_{wl}$	radius of soil water films	m	F6b	
$S$	change in entropy	$J mol^{-1} K^{-1}$	F2	710

$T_l$	soil temperature	K	F2,F8
$U_{\chi i,l}$	uptake of nodule nonstructural C for growth	$\text{g C m}^{-2} \text{ h}^{-1}$	F15,F16,F24
$V_{\chi i,l}$	nonstructural C transfer between root and nodule	$\text{g C m}^{-2} \text{ h}^{-1}$	F21,F24
$V_{\chi i,l}$	nonstructural N transfer between root and nodule	$\text{g N m}^{-2} \text{ h}^{-1}$	F22,F25
$V_{N_2 i,l}$	$\text{N}_2$ fixation	$\text{g N m}^{-2} \text{ h}^{-1}$	F12,F14,F25
$V_{O_2 \text{maxi},l}$	$\text{O}_2$ uptake by nodules under non-limiting $\text{O}_2$	$\text{g O m}^{-2} \text{ h}^{-1}$	F4,F5,F6a
$V_{O_2 i,l}$	$\text{O}_2$ uptake by nodules under ambient $\text{O}_2$	$\text{g O m}^{-2} \text{ h}^{-1}$	F4,F6
$V_{\pi i,l}$	nonstructural P transfer between root and nodule	$\text{g P m}^{-2} \text{ h}^{-1}$	F23,F26
$Y_n'$	nodule growth yield	$\text{g C g C}^{-1}$	F15,F16 0.67
y	shape parameter for $f_{\text{tm}}$	-	F8 0.081

## **S7: CH<sub>4</sub> Production and Consumption**

### *Anaerobic Fermenters and H<sub>2</sub> Producing Acetogens*

The states  $S_{i,j,k}$ ,  $B_{i,k}$  and  $Z_{i,j,k}$  in *ecosys* are substrates for hydrolysis by all active ( $j = a$ ) heterotrophic biomass communities  $M_{i,n,a}$  (Eqs. [1 - 7] of Grant et al., 1993a), which include fermenters plus acetogens. Hydrolysis products are transferred to soluble organic matter  $DOC_{i,k}$  which is the substrate for respiration and uptake by microbial biomass  $M_{i,n,j}$  as described for aerobic heterotrophs in Eq. [11] of Grant et al., (1993a). Respiration  $R_{i,f}$  of  $DOC_{i,c}$  by fermenters plus acetogens ( $n = f$ ) is a Michaelis-Menten function of  $[DOC_{i,c}]$  inhibited by  $O_2$  (Eq. [G1]). Respiration products are partitioned among  $A_{i,c}$ ,  $CO_2$  and  $H_2$  according to Brock and Madigan (1991) (Eq. [G2]).  $R_{i,f}$  beyond that used for maintenance respiration drives the uptake of additional  $DOC_{i,c}$  (Eq. [G3]) for microbial growth according to the growth yield  $Y_f$  of fermentation (Eq. [G4]). The growth yield from fermentation is calculated by dividing the free energy change of fermentation, adjusted for  $H_2$  product concentration (Eq. [G5]), by the energy required to transform soluble organic C into microbial C (Eq. [G4]). Change in  $M_{i,f,j}$  is thus the difference between uptake and respiration of  $DOC_{i,c}$ , less decomposition (Eq. [G6]). This change determines  $M_{i,f,a}$  used in the following calculation of  $R_{i,f}$  (Eq. [G1]). Ratios of  $M_{i,f,j,c}$  to  $M_{i,f,j,n}$  determine mineralization-immobilization of N (Eq. [23] in Grant et al., 1993a). Decomposition products  $D_{i,f,j,k}$  are partitioned to microbial residues  $Z_{i,j,k}$  and soil organic matter  $S_{i,j,k}$  (where  $i$  = passive soil organic matter) ( Eqs. [26-28] in Grant et al., 1993a) which undergo further hydrolysis.

### *Acetotrophic Methanogens*

The fermenter product  $A_{i,c}$  (Eq. [G2]) is the substrate for respiration  $R_{i,m}$  by acetotrophic methanogens ( $n = m$ ) (Eq. [G7]). Respiration products are partitioned between  $CH_4$  and  $CO_2$  according to Brock and Madigan (1991) (Eq. [G8]).  $R_{i,m}$  beyond that used for maintenance respiration drives the uptake of additional  $A_{i,c}$  (Eq. [G9]) for microbial growth according to the growth yield  $Y_m$  of acetotrophic methanogenesis (Eq. [G10]). This growth yield is calculated by dividing the free energy change of acetotrophic methanogenesis (Brock and Madigan, 1991) by the energy required to transform acetate into microbial C. Acetogenic methanogens in the model use acetate as their sole carbon and energy source (Smith and Mah, 1980). Change in  $M_{i,m,j}$  is thus the difference between uptake and respiration of  $A_{i,c}$ , less decomposition (Eq. [G11]). This change determines  $M_{i,m,a}$  used in the following calculation of  $R_{i,m}$  (Eq. [G7]). Mineralization and decomposition processes are the same as those for other microbial populations.

### *Hydrogenotrophic Methanogens*

The fermenter products  $\text{CO}_2$  and  $\text{H}_2$  (Eq. [G2]) are the substrates for  $\text{CO}_2$  reduction by hydrogenotrophic methanogens ( $n = h$ ) which are assumed to be autotrophic (Eq. [G12]). Respiration products are partitioned between  $\text{CH}_4$  and  $\text{H}_2\text{O}$  according to Brock and Madigan (1991) (Eq. [G13]).  $R_h$  beyond that used for maintenance respiration drives the uptake of additional  $\text{CO}_2$  (Eq. [G14]) for microbial growth according to the growth yield  $Y_h$  of hydrogenotrophic methanogenesis (Brock and Madigan, 1991) (Eq. [G15]). This growth yield is calculated by dividing the free energy change of hydrogenotrophic methanogenesis, adjusted for  $\text{H}_2$  substrate concentration (Eq. [G16]), by the energy required to transform  $\text{CO}_2$  into microbial C. Change in  $M_{h,j}$  is thus the difference between uptake and respiration of  $\text{CO}_2$ , less decomposition (Eq. [G17]). This change determines  $M_{h,a}$  used in the following calculation of  $R_h$  (Eq. [G12]). Mineralization and decomposition processes are the same as those for other microbial populations.

#### *Autotrophic Methanotrophs*

Methane generated by acetotrophic and hydrogenotrophic methanogens is the substrate for  $\text{CH}_4$  oxidation by autotrophic methanotrophs ( $n = t$ ) (Eq. [G18]). The stoichiometry and energetics of the methanotrophic reactions (Eqs. [G22 – G24]) are based on those of  $\text{CH}_4$  to  $\text{CO}_2$  in Brock and Madigan (1991). The oxidation of  $\text{CH}_4$  to  $\text{CO}_2$  is coupled through an energy yield with the oxidation of  $\text{CH}_4$  to organic C used in microbial respiration (Eq. [G19]). The energy yield from  $\text{CH}_4$  oxidation is calculated by dividing the free energy change of  $\text{CH}_4$  oxidation by the energy required to transform  $\text{CH}_4$  into organic C (Eq. [G20]). Oxygen requirements to sustain  $\text{CH}_4$  oxidation rates are then calculated from the stoichiometries of  $\text{CH}_4$  oxidation (Eq. [G22 and G23]) and aerobic microbial respiration (Eq. [G24]). The  $\text{O}_2$  concentrations at methanotrophic microsites are then found at which active  $\text{O}_2$  uptake driven by requirements for  $\text{CH}_4$  oxidation equals spherical  $\text{O}_2$  diffusion to the microsites from the soil solution. These microsites are considered to be uniformly distributed on soil surfaces and are separated from the soil atmosphere (if present) by a water film of uniform thickness that depends upon soil water potential. The  $\text{O}_2$  uptake by each aerobic microbial population in the model competes with that by all other aerobic microbial populations (e.g. Grant, 1995; Grant and Rochette, 1994), and is constrained by  $\text{O}_2$  transfer rates through the gaseous and aqueous phases of the soil profile. The ratio of  $\text{O}_2$  uptake to  $\text{O}_2$  requirement  $f_{\text{O}_2 t}$  is then used to constrain  $\text{CH}_4$  oxidation rates (Eq. [G21]) so that  $\text{CH}_4$  oxidation is stoichiometrically coupled to  $\text{O}_2$  uptake. Growth respiration by methanotrophs is calculated as the difference between total respiration  $R_t$  from Eq. [G21b] and maintenance respiration  $R_{\text{mt}}$  from Eqs. [18-19] of Grant et al. (1993a). Growth respiration drives the uptake and transformation of additional  $\text{CH}_4$  into microbial biomass  $M_{t,c}$  (Eq. [G25]) according to the growth yield. This yield is calculated by dividing the free energy change of  $\text{CH}_4$  oxidation (Brock and Madigan, 1991) (Eq. [G18]) by the energy required to construct new microbial biomass from  $\text{CH}_4$  (Eq. [G26]). Net growth of the methanotrophic population  $M_{t,j,c}$  is calculated as the uptake of  $\text{CH}_4 - \text{C}$  minus respiration and decomposition of assimilated C (Eq. [G27]). This change determines  $M_{t,a}$  used in the following calculation of  $X'_t$  (Eq. [G18]). Mineralization and decomposition processes are the same as those for other microbial populations.

This submodel of autotrophic methanotrophy has been used to simulate methanotrophic growth yields, specific growth rates,  $\text{CH}_4$  concentration profiles and the sensitivity of  $\text{CH}_4$  uptake to temperature and water content in soil columns (Grant, 1999). The combined submodels of anaerobic fermentation, acetotrophic methanogenesis, hydrogenotrophic methanogenesis and autotrophic methanotrophy have been used to simulate methanogenic growth yields, specific growth rates, and the time course of  $\text{CH}_4$  emissions from differently amended soil columns at different temperatures (Grant, 1998b). All input parameter values used in Eqs. [G1] to [G27] (Table 1) were derived from the microbiological literature and remain unchanged from those used in Grant (1998b) and in Grant (1999).

**Table S7: CH<sub>4</sub> Production and Consumption**

*Anaerobic Fermenters and H<sub>2</sub> Producing Acetogens*

$R_{i,f} = \{R'_f M_{i,f,a} [Q_{i,c}] / ([Q_{i,c}] + K_f (1 + [O_2] / K_i))\} f_t$	respiration by fermenters	[G1]
$Q_{i,c} \rightarrow 0.67 A_{i,c} + 0.33 CO_2\text{-C} + 0.11 H_2$	partition respiration products	[G2]
$U_{i,f,c} = Rm_{i,f} + (R_{i,f} - Rm_{i,f}) (1.0 + Y_f)$	uptake of DOC by fermenters	$[R_{i,f} > Rm_{i,f}]$ [G3a]
$U_{i,f,c} = R_{i,f}$		$[R_{i,f} < Rm_{i,f}]$ [G3b]
$Y_f = -\Delta G_f / E_M$	growth yield of fermentation	[G4]
$\Delta G_f = \Delta G'_f + \{R T \ln([H_2] / [H_2'])^4\}$	free energy change of fermentation	[G5]
$\delta M_{i,f,j,c} / \delta t = F_j U_{i,f,c} - F_j R_{i,f} - D_{i,f,j,c}$	growth of fermenters	$[R_{i,f} > Rm_{i,f}]$ [G6a]
$\delta M_{i,f,j,c} / \delta t = F_j U_{i,f,c} - R_{mi,f,j} - D_{i,f,j,c}$		$[R_{i,f} < Rm_{i,f}]$ [G6b]

*Acetotrophic Methanogens*

$R_{i,m} = \{R'_m M_{i,m,a} [A_{i,c}] / (K_m + [A_{i,c}])\} f_t$	respiration by acetotrophic methanogens	[G7]
$A_{i,c} \rightarrow 0.50 CH_4\text{-C} + 0.50 CO_2\text{-C}$	partition respiration products	[G8]
$U_{i,m,c} = R_{mi,m} + (R_{i,m} - R_{mi,m}) (1.0 + Y_m)$	uptake by acetotrophic methanogens	$[R_{i,m} > R_{mi,m}]$ [G9a]
$U_{i,m,c} = R_{i,m}$		$[R_{i,m} < R_{mi,m}]$ [G9b]
$-Y_m = -\Delta G'_m / E_M$	growth yield of acetotrophic methanogenesis	[G10]
$\delta M_{i,m,j,c} / \delta t = F_j U_{i,m,c} - F_j R_{i,m} - D_{i,m,j,c}$	growth of acetotrophic methanogens	$[R_{i,m} > R_{mi,m}]$ [G11a]

$$\delta M_{i,m,j,c} / \delta t = F_j U_{i,m,c} - R_{mi,m,j} - D_{i,m,j,c} \quad [R_{i,m} < R_{mi,m}] \quad [G11b]$$

### Hydrogenotrophic Methanogens

$R_h = \{R'_h M_{h,a} [H_2] / (K_h + [H_2]) [CO_2] / (K_c + [CO_2])\} f_t$	respiration by hydrogenotrophic methanogens	[G12]
$CO_2\text{-C} + 0.67 H_2 \rightarrow CH_4\text{-C}$	transform respiration products	[G13]
$U_{h,c} = R_{mh} + (R_h - R_{mh}) (1.0 + Y_h)$	uptake by hydrogenotrophic methanogens	$[R_h > R_{mh}]$ [G14a]
$U_{h,c} = R_h$		$[R_h < R_{mh}]$ [G14b]
$Y_h = -\Delta G_h / E_c$	growth yield of hydrogenotrophic methanogenesis	[G15]
$\Delta G_h = \Delta G'_h - \{R T \ln([H_2] / [H'_2])^4\}$	free energy change of hydrogenotrophic methanogenesis	[G16]
$\delta M_{h,j,c} / \delta t = F_j U_{h,c} - F_j R_h - D_{h,j,c}$	growth of hydrogenotrophic methanogens	$[R_h > R_{mh}]$ [G17a]
$\delta M_{h,j,c} / \delta t = F_j U_{h,c} - R_{mh,j} - D_{h,j,c}$		$[R_h < R_{mh}]$ [G17b]

### Autotrophic Methanotrophs

$X'_t = \{X'_t M_{t,a} [CH_4] / (K_t + [CH_4])\} f_t$	$CH_4$ oxidation by methanotrophs under non-limiting $O_2$	[G18]
$R'_t = X'_t Y_{t_R}$	respiration by methanotrophs under non-limiting $O_2$	[G19]
$Y_{t_R} = -\Delta G'_t / E_G$	energy yield from $CH_4$ oxidation	[G20]
$X_t = X'_t f_{O_2,t}$	$CH_4$ oxidation by methanotrophs under ambient $O_2$	[G21a]
$R_t = R'_t f_{O_2,t}$	respiration by methanotrophs under ambient $O_2$	[G21b]
$CH_4\text{-C} + 4.0 O_2 \rightarrow CO_2\text{-C} + 1.5 H_2O + 0.167 H^+$	$O_2$ requirements for $CH_4$ oxidation by methanotrophs	[G22]
$CH_4\text{-C} + 1.33 O_2 \rightarrow CH_2O\text{-C} + 0.167 H^+$	$O_2$ requirements for growth by methanotrophs	[G23]

$\text{CH}_2\text{O} - \text{C} + 2.67 \text{ O}_2 \rightarrow \text{CO}_2 - \text{C} + 1.5 \text{ H}_2\text{O}$	O <sub>2</sub> requirements for respiration by methanotrophs	[G24]
$U_{t,c} = R_{mt} + (R_t - R_{mt})(1.0 + Y_{t_G})$	uptake by methanotrophs	$[R_t > R_{mt}]$ [G25a]
$U_{t,c} = R_t$		$[R_t < R_{mt}]$ [G25b]
$Y_{t_G} = -\Delta G'_{\text{c}} / E_M$	growth yield of methanotrophy	[G26]
$\delta M_{t,j,c} / \delta t = F_j U_{t,c} - F_j R_t - D_{t,j,c}$		$[R_t > R_{mt}]$ [G27a]
$\delta M_{t,j,c} / \delta t = F_j U_{t,c} - R_{mt,j} - D_{t,j,c}$		$[R_t < R_{mt}]$ [G27b]

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### Definition of Variables in Table S7

Variable	Definition	Units	Equations	Input Values	Reference
A	acetate	g C m <sup>-2</sup>	[G2]		
[A]	aqueous concentration of acetate	g C m <sup>-3</sup>	[G7]		
<i>a</i>	descriptor for <i>j</i> = active component of <i>Mi</i>				
[CH <sub>4</sub> ]	aqueous concentration of CH <sub>4</sub>	g C m <sup>-3</sup>	[G18]		
[CO <sub>2</sub> ]	aqueous concentration of CO <sub>2</sub>	g C m <sup>-3</sup>	[G12]		
D <sub>h,j,c</sub>	decomposition of hydrogenotrophic methanogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G17]		
D <sub>i,f,j,c</sub>	decomposition of fermenters and acetogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G6]		
D <sub>i,m,j,c</sub>	decomposition of acetotrophic methanogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G11]		
D <sub>t,j,c</sub>	decomposition of autotrophic methanotrophs	g C m <sup>-2</sup> h <sup>-1</sup>	[G27]		
E <sub>C</sub>	energy required to construct new M from CO <sub>2</sub>	kJ g C <sup>-1</sup>	[G15]	75	

$E_G$	energy required to transform $\text{CH}_4$ into organic C	$\text{kJ g C}^{-1}$	[G20]	23.5	Anthony (1982)
$E_M$	energy required to construct new M from organic C	$\text{kJ g C}^{-1}$	[G4,G10,G26]	25	
$F_j$	partitioning coefficient for $j$ in $M_{i,n,j}$		[G6,G11,G17,G27]		
$f$	descriptor for fermenters and acetogens in each $M_i$				
$f_{O_2t}$	ratio of $\text{O}_2$ uptake to $\text{O}_2$ requirement for $\text{CH}_4$ oxidation		[G21a,b]		
$f_t$	temperature function for growth-related processes (dimensionless)		[G1,G7,G12]		
$\Delta G'_c$	free energy change of C oxidation- $\text{O}_2$ reduction	$\text{kJ g C}^{-1}$	[G26]	-37.5	Brock and Madigan (1991)
$\Delta G'_f$	free energy change of fermentation plus acetogenesis	$\text{kJ g Q}_{i,c}^{-1}$	[G4,G5]		
$\Delta G'_f$	$\Delta G_f$ when $[\text{H}_2] = [\text{H}_2']$	$\text{kJ g Q}_{i,c}^{-1}$	[G5]	-4.43	Brock and Madigan (1991), Schink (1997)
$\Delta G_h$	free energy change of hydrogenotrophic methanogenesis	$\text{kJ g CO}_2\text{-C}^{-1}$	[G15,G16]		
$\Delta G'_h$	free energy change of hydrogenotrophic methanogenesis when $[\text{H}_2] = [\text{H}_2']$	$\text{kJ g CO}_2\text{-C}^{-1}$	[G16]	-0.27	Brock and Madigan (1991)
$\Delta G'_m$	free energy change of acetotrophic methanogenesis	$\text{kJ g A}_{i,c}^{-1}$	[G10]	-1.03	Brock and Madigan (1991), Schink (1997)
$\Delta G'_t$	free energy change of $\text{CH}_4$ oxidation by methanotrophs	$\text{kJ g CH}_4\text{-C}^{-1}$	[G20]	-9.45	Brock and Madigan (1991)

$[H_2]$	aqueous concentration of $H_2$	$g H m^{-3}$	[G5,G12,G16]	
$[H_2']$	aqueous concentration of $H_2$ when $\Delta G_h = \Delta G'h$ and $\Delta G_f = \Delta G'f$	$g H m^{-3}$	[G5,G16]	$2.0 \times 10^{-4}$
$h$	descriptor for hydrogenotrophic methanogens in each $M_i$			Brock and Madigan (1991)
$i$	descriptor for organic matter-microbe complex ( $i$ = plant residue, manure, particulate OM, or humus)			
$j$	descriptor for structural or kinetic components for each functional type within each $M_i$ (e.g. $a = active$ )			
$K_c$	M-M constant for uptake of $CO_2$ by hydrogenotrophic methanogens	$g C m^{-3}$	[G12]	0.12
$K_f$	M-M constant for uptake of $DOC_{i,c}$ by fermenters and acetogens	$g C m^{-3}$	[G1]	12
$K_i$	inhibition constant for $O_2$ on fermentation	$g O m^{-3}$	[G1]	0.32
$K_h$	M-M constant for uptake of $H_2$ by hydrogenotrophic methanogens	$g H m^{-3}$	[G12]	0.01
$K_m$	M-M constant for uptake of $A_{i,c}$ by acetotrophic methanogens	$g C m^{-3}$	[G7]	12
$K_t$	M-M constant for uptake of $CH_4$ by methanotrophs	$g C m^{-3}$	[G18]	$3 \times 10^{-3}$
$k$	descriptor for elemental fraction within each $j$ ( $j = c, n$ or $p$ )			Conrad (1984)
$M$	microbial communities	$g C m^{-2}$		
$M_h$	hydrogenotrophic methanogen community	$g C m^{-2}$	[G12,G17]	
$M_{i,f}$	fermenter and acetogenic community	$g C m^{-2}$	[G1,G6]	

$M_{i,m}$	acetotrophic methanogen community	$\text{g C m}^{-2}$	[G7,G11]	
$M_t$	autotrophic methanotrophic community	$\text{g C m}^{-2}$	[G18,G27]	
$m$	descriptor for acetotrophic methanogens in each $M_i$			
$Q$	dissolved organic matter (DOC)	$\text{g C m}^{-2}$	[G2]	
$[Q]$	aqueous concentration of DOC	$\text{g C m}^{-3}$	[G1]	
$R$	gas constant	$\text{kJ mol}^{-1} \text{K}^{-1}$	[G5,G16]	$8.3143 \times 10^{-3}$
$R'f$	specific respiration by fermenters and acetogens at saturating $[P_{i,c}]$ , 25 °C and zero water potential	$\text{g C g M}_{i,f,a}^{-1} \text{h}^{-1}$	[G1]	0.1
				Lawrence (1971), Wofford et al. (1986)
$R_h$	$\text{CO}_2$ reduction by hydrogenotrophic methanogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G12,G13,G14,G17,G18]	
$R'h$	specific $\text{CO}_2$ reduction by hydrogenotrophic methanogens at saturating $[\text{H}_2]$ and $[\text{CO}_2]$ , and at 25 °C and zero water potential	$\text{g C g M}_{h,a}^{-1} \text{h}^{-1}$	[G12]	0.12
				Shea et al. (1968), Zehnder and Wuhrmann (1977)
$R_{i,f}$	respiration of hydrolysis products by fermenters and acetogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G1,G2,G3,G6]	
$R_{i,m}$	respiration of acetate by acetotrophic methanogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G7,G8,G9,G11]	
$R'm$	specific respiration by acetotrophic methanogens at saturating $[A_{i,c}]$ , 25 °C and zero water potential	$\text{g C g M}_{i,m,a}^{-1} \text{h}^{-1}$	[G7]	0.20
$R_{mh,j}$	maintenance respiration by hydrogenotrophic methanogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G14,G17]	Smith and Mah (1980)
$R_{mi,f,j}$	maintenance respiration by fermenters and acetogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G3,G6]	
$R_{mi,m,j}$	maintenance respiration by acetotrophic methanogens	$\text{g C m}^{-2} \text{h}^{-1}$	[G9,G11]	

$R_{mt,j}$	maintenance respiration by methanotrophs	$\text{g C m}^{-2} \text{ h}^{-1}$	[G25,G27]	
$R_t$	$\text{CH}_4$ oxidation by methanotrophs for respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[G21b,G23,G24, G25,G27a]	
$R'_t$	$\text{CH}_4$ oxidation by methanotrophs for respiration at saturating $\text{O}_2$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G19,G21b]	
$T$	soil temperature	K	[G5,G16]	
$t$	descriptor for autotrophic methanotrophs			
$U_{h,c}$	rate of $\text{CO}_2$ uptake by $M_h$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G14,G17,G18]	
$U_{i,f,k}$	rate of $\text{DOC}_{i,k}$ uptake by $M_{i,f}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G3,G6]	
$U_{i,m,c}$	rate of $\text{A}_{i,c}$ uptake by $M_{i,m}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G9,G11]	
$U_{t,c}$	rate of $\text{CH}_4$ uptake by $M_t$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G25,G27]	
$X_t$	$\text{CH}_4$ oxidation by methanotrophs	$\text{g C m}^{-2} \text{ h}^{-1}$	[G21a,G22]	
$X'_t$	$\text{CH}_4$ oxidation by methanotrophs at saturating $\text{O}_2$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G1,G2,G4a]	
$X'_t$	specific $\text{CH}_4$ oxidation by methanotrophs at saturating $\text{O}_2$ , 30 °C and zero water potential	$\text{g C g}^{-1} \text{ h}^{-1}$	[G18]	0.5
$Y_f$	biomass yield from fermentation and acetogenic reactions	$\text{g M}_{i,f} \text{ g Q}_{i,c}^{-1}$	[G3,G4]	
$Y_h$	biomass yield from hydrogenotrophic methanogenic reaction	$\text{g M}_h \text{ g CO}_2\text{-C}^{-1}$	[G14,G15,G18]	
$Y_m$	biomass yield from acetotrophic methanogenic reaction	$\text{g M}_{i,m} \text{ g A}_{i,c}^{-1}$	[G9,G10]	
$Y_{t_G}$	biomass yield from methanotrophic growth respiration	$\text{g M}_t\text{-C g CH}_4\text{-C}^{-1}$	[G25a,G26]	
$Y_{t_R}$	ratio of $\text{CH}_4$ respiration vs. $\text{CH}_4$ oxidized by methanotrophs	$\text{g C g C}^{-1}$	[G19,G20]	

Conrad (1984)

## S8: Inorganic N Transformations

### *Mineralization and Immobilization of Ammonium by All Microbial Populations*

Each functional component  $j$  ( $j$  = labile or resistant) of each microbial population  $m$  ( $m$  = obligately aerobic bacteria, obligately aerobic fungi, facultatively anaerobic denitrifiers, anaerobic fermenters plus H<sub>2</sub>-producing acetogens, acetotrophic methanogens, hydrogenotrophic methanogens and methanotrophs, NH<sub>4</sub><sup>+</sup> and NO<sub>2</sub><sup>-</sup> oxidizers, and non-symbiotic diazotrophs) in each substrate-microbe complex  $i$  ( $i$  = animal manure, coarse woody plant residue, fine non-woody plant residue, particulate organic matter, or humus) seeks to maintain a set C:N ratio by mineralizing NH<sub>4</sub><sup>+</sup> ([H1a]) or by immobilizing NH<sub>4</sub><sup>+</sup> ([H1b]) or NO<sub>3</sub><sup>-</sup> ([H1c]). Provision is made for C:N ratios to rise above set values during immobilization, but at a cost to microbial function. These transformations control the exchange of N between organic and inorganic states.

### *Oxidation of DOC and Reduction of Oxygen by Heterotrophs*

Constraints on heterotrophic oxidation of DOC imposed by O<sub>2</sub> uptake are solved in four steps:

- 1) DOC oxidation under non-limiting O<sub>2</sub> is calculated from active biomass and DOC concentration ([H2]),
- 2) O<sub>2</sub> reduction under non-limiting O<sub>2</sub> is calculated from 1) using a set respiratory quotient ([H3]),
- 3) O<sub>2</sub> reduction under ambient O<sub>2</sub> is calculated from radial O<sub>2</sub> diffusion through water films of thickness determined by soil water potential ([H4a]) coupled with active uptake at heterotroph surfaces driven by 2) ([H4b]). O<sub>2</sub> diffusion and active uptake is population-specific, allowing the development of more anaerobic conditions at microbial surfaces associated with more biologically active substrates. O<sub>2</sub> uptake by heterotrophs also accounts for competition with O<sub>2</sub> uptake by nitrifiers, roots and mycorrhizae,
- 4) DOC oxidation under ambient O<sub>2</sub> is calculated from 2) and 3) ([H5]). The energy yield of DOC oxidation drives the uptake of additional DOC for construction of microbial biomass  $M_{i,h}$  according to construction energy costs of each heterotrophic population (Eqs. [7] to [13] in Grant and Pattey, 2003). Energy costs of denitrifiers are slightly larger than those of obligate heterotrophs, placing denitrifiers at a competitive disadvantage for growth and hence DOC oxidation if electron acceptors other than O<sub>2</sub> are not used.

### *Oxidation of DOC and Reduction of Nitrate, Nitrite and Nitrous Oxide by Denitrifiers*

Constraints imposed by NO<sub>3</sub><sup>-</sup> availability on DOC oxidation by denitrifiers are solved in five steps:

- 1)  $\text{NO}_3^-$  reduction under non-limiting  $\text{NO}_3^-$  is calculated from a fraction of electrons demanded by DOC oxidation but not accepted by  $\text{O}_2$  because of diffusion limitations ([H6]),
- 2)  $\text{NO}_3^-$  reduction under ambient  $\text{NO}_3^-$  is calculated from 1) depending on relative concentrations and affinities of  $\text{NO}_3^-$  and  $\text{NO}_2^-$  ([H7]),
- 3)  $\text{NO}_2^-$  reduction under ambient  $\text{NO}_2^-$  is calculated from demand for electrons not met by  $\text{NO}_3^-$  in 2) ([H8]) depending on relative concentrations and affinities of  $\text{NO}_2^-$  and  $\text{N}_2\text{O}$ ,
- 4)  $\text{N}_2\text{O}$  reduction under ambient  $\text{N}_2\text{O}$  is calculated from demand for electrons not met by  $\text{NO}_2^-$  in 3) ([H9]),
- 5) additional DOC oxidation enabled by  $\text{NO}_x$  reduction in 2), 3) and 4) is added to that enabled by  $\text{O}_2$  reduction from [H5], the energy yield of which drives additional DOC uptake for construction of  $M_{i,n}$ . This additional uptake offsets the disadvantage incurred by the larger construction energy costs of denitrifiers.

#### *Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers*

Constraints on nitrifier oxidation of  $\text{NH}_3$  imposed by  $\text{O}_2$  uptake are solved in four steps:

- 1) substrate ( $\text{NH}_3$ ) oxidation under non-limiting  $\text{O}_2$  is calculated from active biomass and from  $\text{NH}_3$  and  $\text{CO}_2$  concentrations ([H11]),
- 2)  $\text{O}_2$  reduction under non-limiting  $\text{O}_2$  is calculated from 1) using set respiratory quotients ([H12]),
- 3)  $\text{O}_2$  reduction under ambient  $\text{O}_2$  is calculated from radial  $\text{O}_2$  diffusion through water films of thickness determined by soil water potential ([H13a]) coupled with active uptake at nitrifier surfaces driven by 2) ([H13b]).  $\text{O}_2$  uptake by nitrifiers also accounts for competition with  $\text{O}_2$  uptake by heterotrophic DOC oxidizers, roots and mycorrhizae,
- 4)  $\text{NH}_3$  oxidation under ambient  $\text{O}_2$  is calculated from 2) and 3) ([H14]). The energy yield of  $\text{NH}_3$  oxidation drives the fixation of  $\text{CO}_2$  for construction of microbial biomass  $M_{i,n}$  according to construction energy costs of each nitrifier population (Eqs. [32] to [34] in Grant and Pattey, 2003).

#### *Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers*

Constraints on nitrifier oxidation of  $\text{NO}_2^-$  imposed by  $\text{O}_2$  uptake ([H15] to [H18]) are solved in the same way as are those of  $\text{NH}_3$  ([H11] to [H14]). The energy yield of  $\text{NO}_2^-$  oxidation drives the fixation of  $\text{CO}_2$  for construction of microbial biomass  $M_{i,o}$  according to construction energy costs of each nitrifier population.

#### *Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers*

Constraints on nitrifier oxidation imposed by  $\text{NO}_2^-$  availability are solved in three steps:

- 1)  $\text{NO}_2^-$  reduction under non-limiting  $\text{NO}_2^-$  is calculated from a fraction of electrons demanded by  $\text{NH}_3$  oxidation but not accepted by  $\text{O}_2$  because of diffusion limitations ([H19]),
- 2)  $\text{NO}_2^-$  reduction under ambient  $\text{NO}_2^-$  and  $\text{CO}_2$  is calculated from step (1) ([H20]), competing for  $\text{NO}_2^-$  with [H18],
- 3) additional  $\text{NH}_3$  oxidation enabled by  $\text{NO}_2^-$  reduction in 2) [H21] is added to that enabled by  $\text{O}_2$  reduction from [H14]. The energy yield from this oxidation drives the fixation of additional  $\text{CO}_2$  for construction of  $M_{i,n}$ .

**Table S8: Inorganic N Transformations**

*Mineralization and Immobilization of Ammonium by All Microbial Populations*

$$I_{\text{NH}_4i,n,j} = (M_{i,m,j,C} C_{Nj} - M_{i,m,j,N}) \quad (I_{\text{NH}_4i,n,j} < 0) \quad [\text{H1a}]$$

$$I_{\text{NH}_4i,n,j} = (M_{i,m,j,C} C_{Nj} - M_{i,m,j,N}) [\text{NH}_4^+] / ([\text{NH}_4^+] + K_{\text{NH}_4m}) \quad (I_{\text{NH}_4i,n,j} > 0) \quad [\text{H1b}]$$

$$I_{\text{NO}_3i,n,j} = (M_{i,m,j,C} C_{Nj} - (M_{i,m,j,N} + I_{\text{NH}_4i,n,j})) [\text{NO}_3^-] / ([\text{NO}_3^-] + K_{\text{NO}_3m}) \quad (I_{\text{NO}_3i,n,j} > 0) \quad [\text{H1b}]$$

*Oxidation of DOC and Reduction of Oxygen by Heterotrophs*

$$X'_{\text{DOC},h} = \{X'_{\text{DOC}} M_{i,h,a} [\text{DOC}_i] / ([\text{DOC}_i]) + K_{Xh}\} f_t \quad [\text{H2}]$$

$$R'_{\text{O}_2i,h} = \mathbf{RQ}_C X'_{\text{DOC},h} \quad [\text{H3}]$$

$$R_{\text{O}_2i,h} = 4\pi n M_{i,h,a} D_{\text{so}_2} ([\text{O}_{2s}] - [\text{O}_{2mi,h}]) [r_m r_w / (r_w - r_m)] \quad [\text{H4a}]$$

$$= R'_{\text{O}_2i,h} [\text{O}_{2mi,h}] / ([\text{O}_{2mi,h}] + K_{\text{O}_2h}) \quad [\text{H4b}]$$

$$X_{\text{DOC},h} = X'_{\text{DOC},h} R_{\text{O}_2i,h} / R'_{\text{O}_2i,h} \quad [\text{H5}]$$

*Oxidation of DOC and Reduction of Nitrate, Nitrite and Nitrous Oxide by Denitrifiers*

$$R'_{\text{NO}_3i,d} = E_{\text{NO}_x} (R'_{\text{O}_2i,d} - R_{\text{O}_2i,d}) \quad [\text{H6}]$$

$$R_{\text{NO}_3i,d} = R'_{\text{NO}_3i,d} [\text{NO}_3^-] / ([\text{NO}_3^-] + K_{\text{NO}_3d}) / (1.0 + ([\text{NO}_2^-] K_{\text{NO}_3d}) / ([\text{NO}_3^-] K_{\text{NO}_2d})) \quad [\text{H7a}]$$

$$R_{\text{NO}_3i,d} = R_{\text{NO}_3i,d} / (1.0 + R_{\text{NO}_3i,d} / (K_e V_{i,d})) \quad [\text{H7b}]$$

$$R_{\text{NO}_2i,d} = (R'_{\text{NO}_3i,d} - R_{\text{NO}_3i,d}) [\text{NO}_2^-] / ([\text{NO}_2^-] + K_{\text{NO}_2d}) / (1.0 + ([\text{N}_2\text{O}] K_{\text{NO}_2d}) / ([\text{NO}_2^-] K_{\text{N}_2\text{O}d})) \quad [\text{H8a}]$$

$$R_{\text{NO}_2i,d} = R_{\text{NO}_2i,d} / (1.0 + R_{\text{NO}_2i,d} / (K_e V_{i,d})) \quad [\text{H8b}]$$

$$R_{\text{N}_2\text{O}_i,d} = 2 (R'_{\text{NO}_3i,d} - R_{\text{NO}_3i,d} - R_{\text{NO}_2i,d}) [\text{N}_2\text{O}] / ([\text{N}_2\text{O}] + K_{\text{N}_2\text{O}d}) \quad [\text{H9a}]$$

$$R_{\text{N}_2\text{O}_i,d} = R_{\text{N}_2\text{O}_i,d} / (1.0 + R_{\text{N}_2\text{O}_i,d} / (K_e V_{i,d})) \quad [\text{H9b}]$$

$$X_{\text{DOC},d} = X_{\text{DOC},d} (\text{from [H5]}) + \mathbf{F}_{\text{NO}_x} (R_{\text{NO}_3i,d} + R_{\text{NO}_2i,d}) + \mathbf{F}_{\text{N}_2\text{O}} R_{\text{N}_2\text{O}_i,d} \quad [\text{H10}]$$

*Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers*

$$X'_{\text{NH}_3i,n} = X'_{\text{NH}_3} M_{i,n,a} \{[\text{NH}_3] / ([\text{NH}_3s] + K_{\text{NH}_3n})\} \{[\text{CO}_2s] / ([\text{CO}_2s] + K_{\text{CO}_2})\} f_t \quad [\text{H11}]$$

$$R'_{\text{O}_2i,n} = \mathbf{RQ}_{\text{NH}_3} X'_{\text{NH}_3i,n} + \mathbf{RQ}_C X'_{\text{C}_i,n} \quad [\text{H12}]$$

$$R_{\text{O}_2i,n} = 4\pi n M_{i,n,a} D_{\text{so}_2} (r_m r_w / (r_w - r_m)) ([\text{O}_{2s}] - [\text{O}_{2mi,n}]) \quad [\text{H13a}]$$

$$= R'_{\text{O}_2i,n} [\text{O}_{2mi,n}] / ([\text{O}_{2mi,n}] + K_{\text{O}_2n}) \quad [\text{H13b}]$$

$$X_{\text{NH}_3i,n} = X'_{\text{NH}_3i,n} R_{\text{O}_2i,n} / R'_{\text{O}_2i,n} \quad [\text{H14}]$$

*Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers*

$$X'_{\text{NO}_2i,o} = X'_{\text{NO}_2} M_{i,o,a} \{[\text{NO}_2^-] / ([\text{NO}_2^-] + K_{\text{NO}_2o})\} \{[\text{CO}_{2s}] / ([\text{CO}_{2s}] + K_{\text{CO}_2})\} f_t \quad [\text{H15}]$$

$$R'_{\text{O}_2i,o} = \mathbf{RQ}_{\text{NO}_2} X'_{\text{NO}_2i,o} + \mathbf{RQ}_C X'_{C,i,o} \quad [\text{H16}]$$

$$R_{\text{O}_2i,o} = 4\pi n M_{i,o,a} D_{\text{SO}_2} (r_m r_w / (r_w - r_m)) ([\text{O}_{2s}] - [\text{O}_{2mi,o}]) \quad [\text{H17a}]$$

$$= R'_{\text{O}_2i,o} [\text{O}_{2mi,o}] / ([\text{O}_{2mi,o}] + K_{\text{O}_2o}) \quad [\text{H17b}]$$

$$X_{\text{NO}_2i,o} = X'_{\text{NO}_2i,o} R_{\text{O}_2i,o} / R'_{\text{O}_2i,o} \quad [\text{H18}]$$

### Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers

$$R'_{\text{NO}_2i,n} = E_{\text{NO}_x} (R'_{\text{O}_2i,n} - R_{\text{O}_2i,n}) \quad [\text{H19}]$$

$$R_{\text{NO}_2i,n} = R'_{\text{NO}_2i,n} \{[\text{NO}_2^-] / ([\text{NO}_2^-] + K_{\text{NO}_2n})\} \{[\text{CO}_{2s}] / ([\text{CO}_{2s}] + K_{\text{CO}_2})\} \quad [\text{H20a}]$$

$$R_{\text{NO}_2i,n} = R_{\text{NO}_2i,n} / (1.0 + R_{\text{NO}_2i,n} / (K_e V_{i,n})) \quad [\text{H20b}]$$

$$X_{\text{NH}_3i,n} = X_{\text{NH}_3i,n} (\text{from [H14]}) + 0.33 R_{\text{NO}_2i,n} \quad [\text{H21}]$$

### Definition of Variables in Table S8

Name	Definition	Units	Equations	Input Values	Reference
<i>Subscripts</i>					
<i>a</i>	active component of $M_{i,m}$				
<i>d</i>	heterotrophic denitrifier population (subset of <i>h</i> )				
<i>h</i>	heterotrophic community (subset of <i>m</i> )				
<i>i</i>	substrate-microbe complex				
<i>j</i>	kinetic components of $M_{i,m}$				
<i>m</i>	all microbial communities				
<i>n</i>	autotrophic ammonia oxidizer population (subset of <i>m</i> )				
<i>o</i>	autotrophic nitrite oxidizer population (subset of <i>m</i> )				
<i>Variables</i>					
$C_N$	maximum ratio of $M_{i,m,j,N}$ to $M_{i,m,j,C}$ maintained by $M_{i,m,j}$	g N g C <sup>-1</sup>	[H1]	0.22 and 0.13 for <i>j</i> = labile and resistant	
$[\text{CO}_{2s}]$	CO <sub>2</sub> concentration in soil solution	g C m <sup>-3</sup>	[H11,H15,H20]		
$[\text{DOC}_i]$	concentration of dissolved decomposition products	g C m <sup>-3</sup>	[H2]		

$D_{\text{SO}_2}$	aqueous dispersivity-diffusivity of $\text{O}_2$	$\text{m}^2 \text{ h}^{-1}$	[H4,H13,H17]	
$E_{\text{NO}_x}$	$e^-$ accepted by $\text{NO}_x$ vs. $\text{O}_2$ when oxidizing DOC	$\text{g N g O}_2^{-1}$	[H6,H19]	$28/32 = 0.875$
$F_{\text{NO}_x}$	$e^-$ donated by C vs. $e^-$ accepted by $\text{NO}_x$ when oxidizing DOC	$\text{g C g N}^{-1}$	[H10]	$12/28 = 0.43$
$F_{\text{N}_2\text{O}}$	$e^-$ donated by C vs. $e^-$ accepted by $\text{N}_2\text{O}$ when oxidizing DOC	$\text{g C g N}^{-1}$	[H10]	$6/28 = 0.215$
$f_t$	temperature function for microbial processes	-	[H2,H11,H15]	See S1
$I_{\text{NH}_4i,n,j}$	mineralization ( $I_{\text{NH}_4i,n,j} < 0$ ) or immobilization ( $I_{\text{NH}_4i,n,j} > 0$ ) of $\text{NH}_4^+$ by $M_{i,n,j,C}$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H1]	
$I_{\text{NO}_3i,n,j}$	immobilization ( $I_{\text{NO}_3i,n,j} > 0$ ) of $\text{NO}_3^-$ by $M_{i,n,j,C}$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H1]	
$K_{\text{CO}_2}$	Michaelis-Menten constant for reduction of $\text{CO}_{2\text{S}}$ by $M_{i,n,a}$ and $M_{i,o,a}$	$\text{g C m}^{-3}$	[H11,H15,H20]	0.15
$K_{\text{NH}_3n}$	M-M constant for oxidation of $\text{NH}_{3\text{S}}$ by nitrifiers	$\text{g N m}^{-3}$	[H11]	0.0002
$K_e$	inhibition constant for electrons not accepted by $\text{O}_2$ and transferred to N oxides	$\text{g N m}^{-3} \text{ h}^{-1}$	[H7,H8,H9,H20]	0.125
$K_{\text{NH}_4m}$	M-M constant for microbial $\text{NH}_4^+$ uptake	$\text{g N m}^{-3}$	[H1]	0.35
$K_{\text{NO}_2d}$	M-M constant for reduction of $\text{NO}_2^-$ by denitrifiers	$\text{g N m}^{-3}$	[H7,H8]	1.4
$K_{\text{NO}_2n}$	M-M constant for reduction of $\text{NO}_2^-$ by nitrifiers	$\text{g N m}^{-3}$	[H20]	1.4
$K_{\text{NO}_2o}$	M-M constant for oxidation of $\text{NO}_2^-$ by nitrifiers	$\text{g N m}^{-3}$	[H15]	3.5
$K_{\text{NO}_3d}$	M-M constant for reduction of $\text{NO}_3^-$ by denitrifiers	$\text{g N m}^{-3}$	[H7,H8]	1.4
$K_{\text{N}_2\text{O}d}$	M-M constant for reduction of $\text{N}_2\text{O}$ by denitrifiers	$\text{g N m}^{-3}$	[H9]	0.028
$K_{\text{O}_2h}$	M-M constant for reduction of $\text{O}_{2\text{s}}$ by heterotrophs	$\text{g O}_2 \text{ m}^{-3}$	[H4b]	0.064
				Griffin (1972)

$K_{O_2n}$	M-M constant for reduction of $O_{2s}$ by $NH_3$ oxidizers	$g O_2 m^{-3}$	[H13b]	0.32	Focht and Verstraete (1977)
$K_{O_2o}$	M-M constant for reduction of $O_{2s}$ by $NO_2^-$ oxidizers	$g O_2 m^{-3}$	[H17b]	0.32	Focht and Verstraete (1977)
$K_{Xh}$	M-M constant for oxidation of DOC by heterotrophs	$g C m^{-3}$	[H2]	12	(McGill et al., 1981)
$M_{i,h,a}$	active biomass of heterotrophs	$g C m^{-2}$	[H2,H7]		
$M_{i,n,a}$	active biomass of $NH_3$ oxidizers	$g C m^{-2}$	[H11,H13]		
$M_{i,m,j,C}$	C biomass of microbial population $M_{i,m,j}$	$g C m^{-2}$	[H1]		
$M_{i,m,j,N}$	N biomass of microbial population $M_{i,m,j}$	$g N m^{-2}$	[H1]		
$M_{i,o,a}$	active biomass of $NO_2^-$ oxidizers	$g C m^{-2}$	[H15,H17]		
$[NH_3s]$	concentration of $NH_3$ in soil solution	$g N m^{-3}$	[H11]		
$[NH_4^+]$	concentration of $NH_4^+$ in soil solution	$g N m^{-3}$	[H1]		
$[NO_2^-]$	concentration of $NO_2^-$ in soil solution	$g N m^{-3}$	[H7,H8,H15,H20]		
$[NO_3^-]$	concentration of $NO_3^-$ in soil solution	$g N m^{-3}$	[H7,H8]		
$[N_2O]$	concentration of $N_2O$ in soil solution	$g N m^{-3}$	[H9]		
$n$	number of microbes	$g^{-1}$	[H13,H17]		
$[O_{2mi,h}]$	$O_2$ concentration at heterotrophic surfaces	$g O_2 m^{-3}$	[H7]		
$[O_{2mi,n}]$	$O_2$ concentration at $NH_3$ oxidizer surfaces	$g O_2 m^{-3}$	[H13]		
$[O_{2mi,o}]$	$O_2$ concentration at $NO_2^-$ oxidizer surfaces	$g O_2 m^{-3}$	[H17]		
$[O_{2s}]$	$O_2$ concentration in soil solution	$g O_2 m^{-3}$	[H7,H13,H17]		
$R_{NO_2i,d}$	$NO_2^-$ reduction by denitrifiers	$g N m^{-2} h^{-1}$	[H8,H9,H10]		
$R'_{NO_2i,n}$	rate of $NO_2^-$ reduction by $NH_3$ oxidizers under non-limiting $[NO_2^-]$ and $[CO_{2s}]$	$g N m^{-2} h^{-1}$	[H19,H20]		
$R_{NO_2i,n}$	rate of $NO_2^-$ reduction by $NH_3$ oxidizers under ambient $[NO_2^-]$ and $[CO_{2s}]$	$g N m^{-2} h^{-1}$	[H20,H21]		
$R'_{NO_3i,d}$	$NO_3^-$ reduction by denitrifiers under non-limiting $[NO_3^-]$	$g N m^{-2} h^{-1}$	[H6,H7,H8,H9]		
$R_{NO_3i,d}$	$NO_3^-$ reduction by denitrifiers under ambient $[NO_3^-]$	$g N m^{-2} h^{-1}$	[H7,H8,H9,H10]		
$R_{N_2Oi,d}$	$N_2O$ reduction by denitrifiers	$g N m^{-2} h^{-1}$	[H9,H10]		

$R'_{O_2i,d}$	rate of $O_2S$ reduction by denitrifiers under non-limiting $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H6]	
$R_{O_2i,d}$	rate of $O_2S$ reduction by denitrifiers under ambient $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H6]	
$R'_{O_2i,h}$	rate of $O_2S$ reduction by heterotrophs under non-limiting $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H3,H4,H5]	
$R_{O_2i,h}$	rate of $O_2S$ reduction by heterotrophs under ambient $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H4,H5]	
$R'_{O_2i,n}$	rate of $O_2S$ reduction by $NH_3$ oxidizers under non-limiting $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H12,H13,H14,H19]	
$R_{O_2i,n}$	rate of $O_2S$ reduction by $NH_3$ oxidizers under ambient $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H13,H14,H19]	
$R'_{O_2i,o}$	rate of $O_2S$ reduction by $NO_2^-$ oxidizers under non-limiting $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H16,H17,H18]	
$R_{O_2i,o}$	rate of $O_2S$ reduction by $NO_2^-$ oxidizers under ambient $[O_{2S}]$	$g O_2 m^{-2} h^{-1}$	[H17,H18]	
$RQ_C$	respiratory quotient for reduction of $O_2$ coupled to oxidation of C	$g O_2 g C^{-1}$	[H3,H12,H16]	2.67
$RQ_{NH_3}$	respiratory quotient for reduction of $O_2$ coupled to oxidation of $NH_3S$	$g O_2 g N^{-1}$	[H12]	3.43
$RQ_{NO_2}$	respiratory quotient for reduction of $O_2$ coupled to oxidation of $NO_2^-$	$g O_2 g N^{-1}$	[H16]	1.14
$r_m$	radius of microbial sphere	m	[H4,H13,H17]	from $\psi_s$ according to Kemper (1966)
$r_w$	radius of $r_m$ + water film at current soil water potential	m	[H4,H13,H17]	
$V_i$	soil water volume occupied by substrate-microbe complex		[7,H8,H9,H20]	
$X'_{C,i,n}$	rate of C oxidation by $NH_3$ oxidizers under non-limiting $[O_{2S}]$	$g C m^{-2} h^{-1}$	[H12]	
$X'_{C,i,o}$	rate of C oxidation by $NO_2^-$ oxidizers under non-limiting $[O_{2S}]$	$g C m^{-2} h^{-1}$	[H16]	

$X'_{\text{DOC}}$	specific rate of DOC oxidation by heterotrophs at 25 °C under non-limiting [DOC] and [O <sub>2S</sub> ]	g C g C <sup>-1</sup> h <sup>-1</sup>	[H2]	0.125	Shields et al. (1973)
$X'_{\text{DOC}i,h}$	rate of DOC oxidation by heterotrophs under non-limiting [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H2,H3,H5]		
$X_{\text{DOC}i,h}$	rate of DOC oxidation by heterotrophs under ambient [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H5]		
$X_{\text{DOC}i,d}$	rate of DOC oxidation by heterotrophs under ambient [O <sub>2S</sub> ] and [NO <sub>x</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H10]		
$X'_{\text{NH}_3}$	specific rate of NH <sub>3</sub> oxidation by NH <sub>3</sub> oxidizers at 25 °C under non-limiting [O <sub>2S</sub> ]	g N g C <sup>-1</sup> h <sup>-1</sup>	[H11]]	0.625	Belser and Schmidt (1980)
$X_{\text{NH}_3i,n}$	rate of NH <sub>3</sub> oxidation by NH <sub>3</sub> oxidizers coupled with reduction of O <sub>2</sub> + NO <sub>2</sub> <sup>-</sup> under ambient [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H14,H21]		
$X'_{\text{NH}_3i,n}$	rate of NH <sub>3</sub> oxidation by NH <sub>3</sub> oxidizers under non-limiting [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H11,H12,H14]		
$X'_{\text{NO}_2i,o}$	rate of NO <sub>2</sub> <sup>-</sup> oxidation by NO <sub>2</sub> <sup>-</sup> oxidizers under non-limiting [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H15,H16,H18]		
$X_{\text{NO}_2i,o}$	rate of NO <sub>2</sub> <sup>-</sup> oxidation by NO <sub>2</sub> <sup>-</sup> oxidizers coupled with reduction of O <sub>2</sub> under ambient [O <sub>2S</sub> ]	g N m <sup>-2</sup> h <sup>-1</sup>	[H18]		
$X'_{\text{NO}_2}$	specific rate of NO <sub>2</sub> <sup>-</sup> oxidation by NO <sub>2</sub> <sup>-</sup> oxidizers at 25 °C under non-limiting [O <sub>2S</sub> ]	g N g C <sup>-1</sup> h <sup>-1</sup>	[H15]	2.5	Belser (1977)

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