

## Supplementary Material

### Introduction

*Ecosys* is a sub-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 is presented in Supplements S1 to S10 below, with reference to equations and variable definitions in Tables S1 to S10. Variables in bold are model inputs with values given in the Definition of Variables associated with each table. These Supplements are:

S1: Microbial C, N and P Transformations

S2: Soil-Plant-Atmosphere Water Relations

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

S4: Soil Water, Heat, Gas and Solute Fluxes

S5: Soil Solute Transformations

S6: Soil and Canopy Symbiotic N<sub>2</sub> Fixation

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

S8: Soil Inorganic N Transformations

S9: Soil Erosion

S10: Canopy and Soil Fire

## **S1: Microbial 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  $D$  is a first-order function of biological activity (represented by heterotrophic respiration  $R_h$ ) of the decomposer biomass  $M$  of all heterotrophic microbial populations [A1]. Decomposer biomasses and their activities are redistributed among complexes according to activity – substrate concentration differences (priming) [A3]. The rate at which each component is hydrolyzed is also a Monod function of substrate concentration [A4], calculated from the fraction of substrate mass colonized by  $M$  [A5]. Hydrolysis rates are controlled by  $T_s$  through an Arrhenius function [A6] and by soil water content ( $\theta$ ) through its effect on aqueous concentrations of heterotrophic activity [ $R_h$ ] [A3,A4] 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 S2 and S4. 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 S3. 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]. Lignin and related hydrolysis products become Particulate Organic Matter (POM).

For decomposition see module ‘C, N, P DECOMPOSITION RATE OF SOLID SUBSTRATES ...’ in nitro.f.

For priming see module ‘PRIMING of DOC,DON,DOP BETWEEN LITTER AND NON-LITTER C’ in nitro.f

For adsorption see module ‘DOC ADSORPTION – DESORPTION’ in nitro.f

### *Microbial Growth*

The DOC product  $Q$  of  $D$  [A1] 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 [A12], DOC,  $T_s$  and water potential  $\psi_s$  [A13] and O<sub>2</sub> [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 S3. 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 NO<sub>3</sub><sup>−</sup>, NO<sub>2</sub><sup>−</sup>, and N<sub>2</sub>O by heterotrophic denitrifiers (S8), and with the reduction of organic C by fermenters and acetotrophic methanogens (S7). In addition, autotrophic nitrifiers conduct NH<sub>4</sub><sup>+</sup> and NO<sub>2</sub><sup>−</sup> oxidation, and NO<sub>2</sub><sup>−</sup> reduction (S8), and autotrophic methanogens and methanotrophs conduct CH<sub>4</sub> production and oxidation (S7).

All microbial populations undergo maintenance respiration  $R_m$  [A18,A19], depending on microbial N and  $T_s$  as described below for plants (S3).  $R_h$  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 remobilization of structural C to nonstructural C to meet excess  $R_m$ , causing microbial senescence.  $M$  also undergoes first-order decay  $D_m$  [A23]. Internal recycling of microbial structural C, N and to nonstructural C, N and P during P senescence and decomposition [A24] is modelled from nonstructural C,N,P ratios. Changes in  $M$  arise from differences between gains from DOC uptake and losses from  $R_m + R_g + D_m$  [A25].

For heterotrophic respiration, see module 'HETEROTROPHIC BIOMASS RESPIRATION' in nitro.f

For energy requirements and yields see parameters 'ENERGY REQUIREMENTS FOR MICROBIAL GROWTH AND ENERGY YIELDS FROM REDUCTION OF O<sub>2</sub>, OC, CH<sub>4</sub>, NO<sub>3</sub>, N<sub>2</sub>' in nitro.f

For O<sub>2</sub> uptake, see module 'O<sub>2</sub> UPTAKE BY AEROBES' in nitro.f

For denitrification, see module 'HETEROTROPHIC DENITRIFICATION' in nitro.f

For fermentation, see module 'RESPIRATION BY HETEROTROPHIC ANAEROBES' in nitro.f

For acetotrophic methanogenesis, see module 'RESPIRATION RATES BY ACETOTROPHIC METHANOGENS' in nitro.f

For autotrophic nitrifiers, methanotrophs and methanogens see modules 'RESPIRATION RATES BY AUTOTROPHS' and 'AUTOTROPHIC DENITRIFICATION' in nitro.f

For microbial decay see module 'MICROBIAL DECOMPOSITION FROM BIOMASS, SPECIFIC DECOMPOSITION' in nitro.f

For microbial C,N,P recycling see module 'RECYCLE C,N,P FROM SENESCING BIOMASS TO NONSTRUCTURAL STORAGE' in nitro.f

### *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  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ ,  $\text{H}_2\text{PO}_4^-$  and  $\text{HPO}_4^{2-}$  [A26], thereby controlling solution  $[\text{NH}_4^+]$ ,  $[\text{NO}_3^-]$ ,  $[\text{H}_2\text{PO}_4^-]$  and  $[\text{HPO}_4^{2-}]$  that determine root and mycorrhizal uptake in S3. 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]. Changes in microbial C, N and P arise from DOC, DON and DOP uptake plus  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ ,  $\text{H}_2\text{PO}_4^-$  and  $\text{HPO}_4^{2-}$  immobilization and N<sub>2</sub> fixation, less  $\text{NH}_4^+$ ,  $\text{NO}_3^-$ , and  $\text{H}_2\text{PO}_4^-$  mineralization and microbial C, N and P decomposition [A29].

For mineralization-immobilization see module 'N AND P MINERALIZATION-IMMOBILIZATION' in nitro.f

For microbial net C, N and P growth see module 'DOC, DON, DOP AND ACETATE UPTAKE DRIVEN BY GROWTH RESPIRATION' in nitro.f

### *Non-symbiotic N<sub>2</sub> Fixation*

Non-symbiotic heterotrophic diazotrophs can also fix aqueous N<sub>2</sub> to maintain their set minimum C:N if immobilization is inadequate [A26], but at an additional respiration cost. N<sub>2</sub> fixation is driven by diazotroph N deficits [A27a] constrained by diazotroph growth respiration such that under large N deficits most growth respiration drives N<sub>2</sub> fixation, while under small N deficits, most growth respiration drives diazotrophic growth [A27b]. Respiration required for N<sub>2</sub> fixation  $R_{\text{N}_2}$  [A27b] is subtracted from  $R_g$  [A20] when calculating diazotrophic growth.

For nonsymbiotic N<sub>2</sub> fixation see module ‘N<sub>2</sub> FIXATION FROM GROWTH RESPIRATION’ in nitro.f

### *Humification*

Microbial 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]. Some microbial senescence and decomposition products [A23,A25] are recycled to microbial nonstructural C,N,P [A24], and the rest are transferred to the humus complex or to microbial residues in the originating complex according to soil clay content [A35–A39]. N:C and P:C ratios in these transfers [A36 vs A35 and A39 vs A38] vary with N and P recycling coefficients [A23b], driven by N:C and P:C ratios in microbial nonstructural pools [A24b] caused by DON:DOC and DOP:DOC ratios from N:C and P:C in organic substrates.

For POM formation see module ‘HUMIFICATION OF DECOMPOSED RESIDUE LIGNIN ...’ in nitro.f.

For humus formation see module ‘HUMIFICATION OF MICROBIAL DECOMPOSITION PRODUCTS’ in nitro.f.

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

	<i>Decomposition</i>	
$D_{Si,j,l,C} = D'_{Si,j,l,C} R_{hi,d,l} f_{igl} (S_{i,j,l,C} / G_{i,l,C})$	decomposition of colonized litter, POC, humus	[A1a]
$D_{Zi,j,l,C} = D'_{Zi,j,l,C} R_{hi,d,l} f_{igl} (Z_{i,j,l,C} / G_{i,l,C})$	decomposition of microbial residues	[A1b]
$D_{Ai,l,C} = D'_{Ai,l,C} R_{hi,d,l} f_{igl} (A_{i,l,C} / G_{i,l,C})$	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]
$R_{hi,n,l} = R_{hi,n,l} + \sum_{ix} q_m (R_{hi,n,l} G_{ix,l,C} - R_{hi,x,n,l} G_{i,l,C}) / (G_{ix,l,C} + G_{i,l,C})$	redistribution of heterotrophic activity by each population $n$ from each substrate-microbe complex $i$ to other complexes $ix$ (priming)	[A3a] [A3b]
$R_{hi,d,l} = \sum_n R_{hi,n,l}$	aqueous concentration of heterotrophic activity	[A3c]
$[R_{hi,d,l}] = R_{hi,d,l} / \theta$		
$D'_{Si,j,l,C} = \{D_{Sj,C} [S_{i,j,l,C}]\} / \{[S'_{i,j,l,C}] + K_{mD} (1.0 + [R_{hi,d,l}] / K_{iD})\}$	substrate and water constraint on $D$ from colonized litter, POC and	[A4a]
$D'_{Zi,j,l,C} = \{D_{Zj,C} [Z_{i,j,l,C}]\} / \{[Z_{i,j,l,C}] + K_{mD} (1.0 + [R_{hi,d,l}] / K_{iD})\}$	humus, microbial residues and adsorbed SOC	[A4b]
$D'_{Ai,l,C} = \{D_{A,C} [A_{i,l,C}]\} / \{[A_{i,l,C}] + K_{mD} (1.0 + [R_{hi,d,l}] / K_{iD})\}$		[A4c]
$S_{i,j,l,C} = \min\{S_{i,j,l,C} + \beta \sum_n R_{hi,n,l} (S_{i,j,l,C} / S'_{i,l,C}), S'_{i,l,C}\}$	colonized litter increases with microbial growth into uncolonized litter	[A5]

$f_{\text{igl}} = T_{\text{sl}} \{ e^{[B_g - H_a / (R T_{\text{sl}})]} \} / \{ 1 + e^{[(H_{\text{dl}} - ST_{\text{sl}}) / (R T_{\text{sl}})]} + e^{[(ST_{\text{sl}} - H_{\text{dh}}) / (R T_{\text{sl}})]} \}$	Arrhenius function for $D$ and $R_h$	[A6]
$D_{S_{i,j,l,N,P}} = D_{S_{i,j,l,C}} (S_{i,j,l,N,P} / S_{i,j,l,C})$	decomposition of N and P are driven by	[A7a]
$D_{Z_{i,j,l,N,P}} = D_{Z_{i,j,l,C}} (Z_{i,j,l,N,P} / Z_{i,j,l,C})$	of C in colonized litter, POC, humus, microbial residues and adsorbed SOC	[A7b]
$D_{A_{i,l,N,P}} = D_{A_{i,l,C}} (A_{i,l,N,P} / A_{i,l,C})$		[A7c]
$Y_{i,l,C} = k_{\text{ts}} (G_{i,l,C} F_s [Q_{i,l,C}]^b - V_{i,l,C})$	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	[A9]
$Y_{i,l,N,P} = Y_{i,l,C} (V_{i,l,N,P} / V_{i,l,C})$	$(Y_{i,l,C} < 0)$ desorption of DON, DOP	[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]
$R'_{hi,n,l} = M_{i,n,a,l,C} \{R_{hi,n,l} [Q_{i,l,C}] / \{ (K_m Q_C + [Q_{i,l,C}]) \} f_{\text{igl}} f_{\psi_{\text{gl}}}$	$R_h$ constrained by substrate DOC, $T_s$ and $\psi$	[A13]
$R_{hi,n,l} = R'_{hi,n,l} (U_{O2i,n,l} / U'_{O2i,n,l})$	$R_h$ constrained by $O_2$	[A14]
$f_{\psi_{\text{gl}}} = e^{(\sigma \psi_s)}$	$\psi_s$ constraints on microbial growth	[A15]
$U'_{O2i,n,l} = 2.67 R'_{hi,n,l}$	$O_2$ 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]
$R_{mi,n,j,l} = R_m M_{i,n,j,l,N} f_{\text{uml}}$	maintenance respiration	[A18]
$f_{\text{uml}} = T_{\text{sl}} \{ e^{[B_m - H_a / (R T_{\text{sl}})]} \} / \{ 1 + e^{[(H_{\text{dl}} - ST_{\text{sl}}) / (R T_{\text{sl}})]} \}$	Arrhenius function for $R_m$	[A19]
$R_{gi,n,l} = R_{hi,n,l} - \sum_j R_{mi,n,j,l} - R_{\Phi_{i,n=f,j,l}}$	growth respiration	[A20]
$Y_g = -\Delta G_x / E_m$	growth yield of aerobic heterotrophs	[A21a]
$U_{i,n,l,C} = \min(R_{hi,n,l}, \sum_j R_{mi,n,j,l}) + R_{gi,n,l} (1 + Y_g)$	DOC uptake driven by $R_g$	[A21b]
$U_{i,n,l,N,P} = U_{i,n,l} Q_{i,l,N,P} / Q_{i,l,C}$	DON, DOP uptake driven by $U_{i,n,l,C}$	[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]
$D_{Mi,n,j,N,P} = D_{Mi,j} M_{i,n,j,l,N,P} (1.0 - X_{N,P} f_{\lambda N,Pi,n,j,l})$	decay of microbial N, P less internal recycling	[A23b]
$f_{\lambda Ci,n,j,l} = \min\{M_{i,n,n,l,N} / (M_{i,n,n,l,N} + M_{i,n,n,l,C} K_{\lambda N}), M_{i,n,n,l,P} + M_{i,n,n,l,C} K_{\lambda P}\}$	internal C,N,P recycling determined by nonstructural C,N,P ratios	[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]
$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,l,C} - F_j R_{hi,n,l} - D_{Mi,n,j,l,C}$	$[R_{hi,n,l} > R_{mi,n,j,l}]$ microbial growth	[A25a]
$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,l,C} - R_{mi,n,j,l} - D_{Mi,n,j,l,C}$	$[R_{hi,n,l} < R_{mi,n,j,l}]$ microbial senescence	[A25b]

## Microbial Nutrient Exchange

$U_{\text{NH}_4 i, n, j, l} = (M_{i, n, j, l, C} \text{ C}_{\text{Nj}} - M_{i, n, j, l, N})$	$U_{\text{NH}_4} < 0$	net mineralization	[A26a]
$U_{\text{NH}_4 i, n, j, l} = \min \{ (M_{i, n, j, l, C} \text{ C}_{\text{Nj}} - M_{i, n, j, l, N}),$ $U'_{\text{NH}_4} a_{i, n, j, l} ([\text{NH}_4^+_{i, n, j, l}] - [\text{NH}_4^+_{\text{mn}}])$ $/ ([\text{NH}_4^+_{i, n, j, l}] - [\text{NH}_4^+_{\text{mn}}] + K_{\text{NH}_4}) \}$	$U_{\text{NH}_4} > 0$		[A26b]
$U_{\text{NO}_3 i, n, j, l} = \min \{ (M_{i, n, j, l, C} \text{ C}_{\text{Nj}} - (M_{i, n, j, l, N} + U_{\text{NH}_4 i, n, j, l})),$ $U'_{\text{NO}_3} a_{i, n, j, l} ([\text{NO}_3^-_{i, n, j, l}] - [\text{NO}_3^-_{\text{mn}}])$ $/ ([\text{NO}_3^-_{i, n, j, l}] - [\text{NO}_3^-_{\text{mn}}] + K_{\text{NO}_3}) \}$	$U_{\text{NO}_3} > 0$	net immobilization	[A26c]
$U_{\text{H}_2\text{PO}_4 i, n, j, l} = (M_{i, n, j, l, C} \text{ C}_{\text{Pj}} - M_{i, n, j, l, P})$	$U_{\text{H}_2\text{PO}_4} < 0$	net mineralization	[A26d]
$U_{\text{H}_2\text{PO}_4 i, n, j, l} = \min \{ (M_{i, n, j, l, C} \text{ C}_{\text{Pj}} - M_{i, n, j, l, P}),$ $U'_{\text{PO}_4} A_{i, n, j, l} ([\text{H}_2\text{PO}_4^-_{i, n, j, l}] - [\text{H}_2\text{PO}_4^-_{\text{mn}}])$ $/ ([\text{H}_2\text{PO}_4^-_{i, n, j, l}] - [\text{H}_2\text{PO}_4^-_{\text{mn}}] + K_{\text{PO}_4}) \}$	$U_{\text{H}_2\text{PO}_4} > 0$	net immobilization	[A26e]
$U_{\text{HPO}_4 i, n, j, l} = \min \{ (M_{i, n, j, l, C} \text{ C}_{\text{Pj}} - (M_{i, n, j, l, P} + U_{\text{H}_2\text{PO}_4 i, n, j, l})),$ $U'_{\text{PO}_4} A_{i, n, j, l} ([\text{HPO}_4^{2-}_{i, n, j, l}] - [\text{HPO}_4^{2-}_{\text{mn}}])$ $/ ([\text{HPO}_4^{2-}_{i, n, j, l}] - [\text{HPO}_4^{2-}_{\text{mn}}] + K_{\text{PO}_4}) \}$	$U_{\text{HPO}_4} > 0$	net immobilization	[A26f]

### Non-symbiotic N<sub>2</sub> Fixation

$R\phi'_{i, n= f, j, l} = \max \{ 0, (M_{i, n= f, j, l, C} \text{ C}_{\text{Nj}} - M_{i, n= f, j, l, N}) / E_{\phi} \}$	maximum respiration of N <sub>2</sub> fixation from diazotrophic N deficit	[A27a]
$R\phi_{i, n= f, j, l} = R_{\text{gi}, n= f, l} R\phi'_{i, n= f, j, l} / (R_{\text{gi}, n= f, l} + R\phi'_{i, n= f, j, l})$	actual respiration of N <sub>2</sub> fixation from diazotrophic growth respiration	[A27b]
$\Phi_{i, n= f, j, l} = E_{\phi} R\phi_{i, n= f, j, l}$	N <sub>2</sub> fixation from N <sub>2</sub> energy yield	[A28]
$\delta M_{i, n, j, l, N} / \delta t = F_j U_{i, n, l, N} + U_{\text{NH}_4 i, n, j, l} + U_{\text{NO}_3 i, n, j, l} + \Phi_{i, n= f, j, l} - D_{M_{i, n, j, l, N}}$	growth vs. losses of microbial N	[A29a]
$\delta M_{i, n, j, l, P} / \delta t = F_j U_{i, n, l, P} + U_{\text{H}_2\text{PO}_4 i, n, j, l} + U_{\text{HPO}_4 i, n, j, l} - D_{M_{i, n, j, l, P}}$	growth vs. losses of microbial P	[A29b]
$M_{i, n, a, l, C} = M_{i, n, j= \text{labile}, l, C} + M_{i, n, j= \text{resistant}, l, C} F_r / F_l$	active microbial biomass calculated from labile fraction	[A30a]

### Humification

$H_{\text{Si}, j= \text{lignin}, l, C} = D_{\text{Si}, j= \text{lignin}, l, C}$	decomposition products of litter substrate added to POC depending on lignin	[A31]
$H_{\text{Si}, j= \text{lignin}, l, N, P} = D_{\text{Si}, j= \text{lignin}, l, N, P}$		[A32]
$H_{\text{Si}, j \neq \text{lignin}, l, C} = H_{\text{Si}, j= \text{lignin}, l, C} L_{\text{hj}}$		[A33]
$H_{\text{Si}, j \neq \text{lignin}, l, N, P} = H_{\text{Si}, j \neq \text{lignin}, l, C} S_{i, l, N, P} / S_{i, l, C}$		[A34]
$H_{M_{i, n, j, l, C}} = D_{M_{i, n, j, l, C}} F_{\text{h}}$	fraction of microbial decay products added to humus	[A35]
$H_{M_{i, n, j, l, N, P}} = H_{M_{i, n, j, l, C}} M_{i, n, j, l, N, P} / M_{i, n, j, l, C}$		[A36]

$F_{\mathbf{h}} = 0.25 + 0.25 F_{\text{clay}}$	fraction of $D_M$ added to humus depends on clay	[A37]
$H_{Zi,n,j,l,C} = D_{Mi,n,j,l,C} - H_{Mi,n,j,l,C}$	remainder of microbial decay products added to microbial residues	[A38]
$H_{Zi,n,j,l,N,P} = D_{Mi,n,j,l,N,P} - H_{Mi,n,j,l,N,P}$		[A39]

## Definition of Variables in Table S1

Variable	Definition	Unit	Equation	Value
<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), diazotrophs, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)			
<i>variables</i>				
$A_{i,l,C}$	mass of adsorbed SOC	g C m <sup>-2</sup>	[A1c,A2c]	
$[A_{i,l,C}]$	concentration of adsorbed SOC in soil	g C Mg <sup>-1</sup>	[A4c]	
<i>a</i>	microbial surface area	m <sup>2</sup> m <sup>-2</sup>	[A26]	
<b>B<sub>g</sub></b>	parameter such that $f_g = 1.0$ at $T_l = 298.15$ K		[A6]	25.229
<b>B<sub>m</sub></b>	parameter such that $f_m = 1.0$ at $T_l = 298.15$ K		[A6]	25.216
<i>b</i>	Freundlich exponent for sorption isotherm		[A8]	0.85
<b>β</b>	specific colonization rate of uncolonized substrate	g C g C <sup>-1</sup> l	[A5]	0.25
$C_{N,Pi,n,a,l}$	ratio of $M_{i,n,a,N,P}$ to $M_{i,n,a,C}$	g N or P g C <sup>-1</sup>	[A12]	
$C_{N,Pj}$	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 <i>j</i> = labile and resistant, respectively
$D_{Ai,l,C}$	decomposition rate of $A_{i,l,C}$ by $R_{hi,d,l}$	g C m <sup>-2</sup> h <sup>-1</sup>	[A1c,A7c,A31c]	
$D_{Aj,C}$	specific decomposition rate of $A_{i,l,C}$ by $R_{hi,d,l}$ at 25°C and saturating $[A_{i,l,C}]$	g C g C <sup>-1</sup> h <sup>-1</sup>	[A4c]	0.25
$D_{Ai,j,l,N,P}$	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]	
$D'_{Ai,j,l,C}$	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]	



$D_{Mi,j}$	specific decomposition rate of $M_{i,n,j}$ at 25°C	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A23a,b]	$1.0 \times 10^{-2}$ and $1.0 \times 10^{-3}$ for $j =$ labile and resistant, respectively	
$D_{Mi,n,j,l,C}$	decomposition rate of $M_{i,n,j,l,C}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[A23a,A25,A35,A38]		
$D_{Mi,n,j,l,N,P}$	decomposition rate of $M_{i,n,j,l,N,P}$	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A23b,A29,A39]		
$D_{Si,j,l,C}$	decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing $Q$ in [A13]	$\text{g C m}^{-2} \text{ h}^{-1}$	[A1a,A7a,A31]		
$D_{Sj,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $R_{hi,d,l}$ at 25°C and saturating $[S_{i,l,C}]$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A4a]	6.75, 6.75, 1.35, and 0.45 for $j =$ protein, carbohydrate, cellulose, and lignin, 0.045 for POC, and 0.045 and 0.015 for active and passive humus.	
$D_{Si,j,l,N,P}$	decomposition rate of $S_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A7a, A32]		
$D'_{Si,j,l,C}$	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]		
$D_{Zi,j,l,C}$	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]		
$D_{Zi,j,l,N,P}$	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]		
$D_{Zj,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $R_{hi,d,l}$ at 25°C and saturating $[Z_{i,l,C}]$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A4b]	6.75 and 1.35 for $j =$ labile and resistant biomass residue	
$D'_{Zi,j,l,C}$	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 ( $n = f$ )	$\text{g N g C}^{-1}$	[A27,A28]	0.25	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]		Sørensen (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]		
$f_{\lambda Ci,n,j,l}$	fraction of C recycled to nonstructural pool during decomposition	-	[A23a,A24a]		
$f_{\lambda N,Pi,n,j,l}$	fraction of N or P recycled to nonstructural pool during decomposition	-	[A23b,A24b]		
$f_{igl}$	temperature function for microbial growth respiration	-	[A1,A6,A13]		
$f_{tml}$	temperature function for maintenance respiration	-	[A18,A19]		
$f_{\nu gl}$	soil water potential function for microbial, root or mycorrhizal growth respiration		[A13,A15]		Pirt (1975)
$\Phi_{i,n=f,j,l}$	non-symbiotic $N_2$ fixation by heterotrophic diazotrophs ( $n = f$ )	$g\ N\ m^{-2}\ h^{-1}$	[A28]		
$G_{i,l,C}$	total C in substrate-microbe complex	$g\ C\ Mg^{-1}$	[A1,A2c,A3a,A8,A37]		
$[H_2PO_4^-]$	concentration of $H_2PO_4^-$ in soil solution	$g\ P\ m^{-3}$	[A26]		
$H_a$	energy of activation	$J\ mol^{-1}$	[A6,A19,C10]	$62.5 \times 10^3$	Addiscott (1983)
$H_{dh}$	energy of high temperature deactivation	$J\ mol^{-1}$	[A6,C10]	$222.5 \times 10^3$	
$H_{dl}$	energy of low temperature deactivation	$J\ mol^{-1}$	[A6,A19,C10]	$197.5 \times 10^3$	
$H_{Mi,n,j,l,C}$	transfer of microbial C decomposition products to humus	$g\ C\ m^{-2}\ h^{-1}$	[A35,A36,A38]		
$H_{Mi,n,j,l,N,P}$	transfer of microbial N or P decomposition products to humus	$g\ N\ or\ P\ m^{-2}\ h^{-1}$	[A36,A39]		
$H_{Si,j,l,C}$	transfer of C hydrolysis products to particulate OM	$g\ C\ m^{-2}\ h^{-1}$	[A31,A33,A34]		
$H_{Si,j,l,N,P}$	transfer of N or P hydrolysis products to particulate OM	$g\ N\ or\ P\ m^{-2}\ h^{-1}$	[A32,A34]		
$H_{Zi,n,j,l,C}$	transfer of microbial C decomposition products to microbial residue	$g\ C\ m^{-2}\ h^{-1}$	[A38]		
$H_{Zi,n,j,l,N,P}$	transfer of microbial N or P decomposition products to microbial residue	$g\ N\ or\ P\ m^{-2}\ h^{-1}$	[A39]		
$K_{\lambda N}$	inhibition constant for internal recycling of C, N	$g\ N\ g\ C^{-1}$	[A24a,b]	0.1	
$K_{\lambda P}$	inhibition constant for internal recycling of C, P	$g\ P\ g\ C^{-1}$	[A24a,b]	0.01	
$K_{iS}$	inhibition constant for microbial colonization of substrate	-	[A5]	0.5	Grant et al. (2010)
$K_{NH_4}$	M-M constant for $NH_4^+$ uptake at microbial surfaces	$g\ N\ m^{-3}$	[A26]	0.40	
$K_{NO_3}$	M-M constant for $NO_3^-$ uptake at microbial surfaces	$g\ N\ m^{-3}$	[A26]	0.35	
$K_{PO_4}$	M-M constant for $H_2PO_4^-$ uptake at microbial surfaces	$g\ P\ m^{-3}$	[A26]	0.125	
$K_{iD}$	inhibition constant for $[R_{hi,d,l}]$ on decomposition of $S_{i,C}$ , $Z_{i,C}$	$g\ C\ m^{-3}\ h^{-1}$	[A4]	2.5	Grant et al. (1993a,b); Lizama and Suzuki (1990)
$K_{mD}$	Michaelis–Menten constant for $D_{Si,j,C}$	$g\ C\ Mg^{-1}$	[A4]	75	

$K_{mQ_C}$	Michaelis–Menten constant for $R'_{hi,n}$ on $[Q_{i,C}]$	$\text{g C m}^{-3}$	[A13]	12	
$K_{O_2}$	Michaelis–Menten constant for reduction of $O_{2s}$ 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 $j = \text{protein, carbohydrate, and cellulose}$	Shulten and Schnitzer (1997)
$M$	molecular mass of water	$\text{g mol}^{-1}$	[A15]	18	
$M_{i,n,j,l,C}$	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 microsities	$\text{m}^{-2}$	[A17b]		
$[\text{NH}_4^+_{i,n,j,l}]$	concentration of $\text{NH}_4^+$ at microbial surfaces	$\text{g N m}^{-3}$	[A26b]		
$[\text{NH}_4^+_{mn}]$	concentration of $\text{NH}_4^+$ at microbial surfaces below which $U_{\text{NH}_4} = 0$	$\text{g N m}^{-3}$	[A26b]	0.0125	
$[\text{NO}_3^-_{i,n,j,l}]$	concentration of $\text{NO}_3^-$ at microbial surfaces	$\text{g N m}^{-3}$	[A26c]		
$[\text{NO}_3^-_{mn}]$	concentration of $\text{NO}_3^-$ at microbial surfaces below which $U_{\text{NO}_3} = 0$	$\text{g N m}^{-3}$	[A26c]	0.03	
$[\text{H}_2\text{PO}_4^-_{i,n,j,l}]$	concentration of $\text{H}_2\text{PO}_4^-$ at microbial surfaces	$\text{g P m}^{-3}$	[A26e]		
$[\text{H}_2\text{PO}_4^-_{mn}]$	concentration of $\text{H}_2\text{PO}_4^-$ at microbial surfaces below which $U_{\text{H}_2\text{O}_4} = 0$	$\text{g P m}^{-3}$	[A26e]	0.002	
$[\text{HPO}_4^{2-}_{i,n,j,l}]$	concentration of $\text{HPO}_4^{2-}$ at microbial surfaces	$\text{g P m}^{-3}$	[A26f]		
$[\text{HPO}_4^{2-}_{mn}]$	concentration of $\text{HPO}_4^{2-}$ at microbial surfaces below which $U_{\text{HPO}_4} = 0$	$\text{g P m}^{-3}$	[A26f]	0.002	
$Q_{i,l,C}$	$DOC$ from products of $D_{Si,j,l,C}$ [A3] and $D_{Zi,j,l,C}$ [A5]	$\text{g C m}^{-2}$	[A8,A13,A22]		
$[Q_{i,l,C}]$	solution concentration of $Q_{i,l,C}$	$\text{g C Mg}^{-1}$	[A8,A13]		
$Q_{i,l,N,P}$	$DON$ 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,A19,C10]	8.3143	

$R'_{\phi_{i,n=f,j,l}}$	maximum respiration for non-symbiotic N <sub>2</sub> fixation by heterotrophic diazotrophs ( $n = f$ )	$\text{g C m}^{-2} \text{ h}^{-1}$	[A27]		
$R_{\phi_{i,n=f,j,l}}$	actual respiration for non-symbiotic N <sub>2</sub> fixation by heterotrophic diazotrophs ( $n = f$ )	$\text{g C m}^{-2} \text{ h}^{-1}$	[A20,A27,A28]		
$R_{gi,l}$	growth respiration of $M_{i,n,a,l}$ on $Q_{i,l,C}$ under nonlimiting O <sub>2</sub> 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, O <sub>2</sub> , nutrients, $\theta$ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A11]		
$R_{hi,d,l}$	heterotrophic activity (respiration) used for decomposition	$\text{g C m}^{-2} \text{ h}^{-1}$	[A1,A3,A4]		
$R_{hi,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under ambient DOC, O <sub>2</sub> , 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 O <sub>2</sub> , DOC, $\theta$ and 25°C	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A12,A13]		
$R'_h{}_n$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting DOC, O <sub>2</sub> , nutrients, $\theta$ and 25°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 <sub>2</sub> and ambient DOC, nutrients, $\theta$ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A13,A14,A16]		
$R_m$	specific maintenance respiration at 25°C	$\text{g C g N}^{-1} \text{ h}^{-1}$	[A18]	0.01	Barnes et al. (1998)
$R_{mi,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[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]	$1.0 \times 10^{-6}$	
$r_{wl}$	thickness of water films	m	[A17]		
$S$	change in entropy	$\text{J mol}^{-1} \text{ K}^{-1}$	[A6,C10]	710	Sharpe and DeMichelle (1977)
$[S_{i,j,l,C}]$	concentration of $S_{i,j,l,C}$ in soil	$\text{g C Mg}^{-1}$	[A4a]		
$S'_{i,j,l,C}$	mass of litter, POC or humus C	$\text{g C m}^{-2}$	[A2a,A5]		
$S_{i,j,l,C}$	mass of colonized litter, POC or humus C	$\text{g C m}^{-2}$	[A1a,A5,A7a,A34]		
$S_{i,j,l,N,P}$	mass of litter, POC or humus N or P	$\text{g N or P m}^{-2}$	[A7a,A34]		
$T_{sl}$	soil temperature	K	[A6,A15.A19]		
$\theta$	soil water content	$\text{m}^3 \text{ m}^{-2}$	[A3c]		
$U_{i,n,l,C}$	uptake of $Q_{i,l,C}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	$\text{g C m}^{-2} \text{ h}^{-1}$	[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	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A22,A29]		
$U_{\text{NH4},i,n,j,l}$	NH <sub>4</sub> <sup>+</sup> uptake by microbes	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26,A27,A29]		
$U'_{\text{NH4}}$	maximum $U_{\text{NH4}}$ at 25 °C and non-limiting NH <sub>4</sub> <sup>+</sup>	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26]	$5.0 \times 10^{-3}$	
$U_{\text{NO3},i,n,j,l}$	NO <sub>3</sub> <sup>-</sup> uptake by microbes	$\text{g N m}^{-2} \text{ h}^{-1}$	[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]	$5.0 \times 10^{-3}$
$U_{\text{O}_2 i,n}$	$\text{O}_2$ uptake by $M_{i,n,a,l}$ under ambient $\text{O}_2$	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A17]	
$U'_{\text{O}_2 i,n}$	$\text{O}_2$ uptake by $M_{i,n,a,l}$ under nonlimiting $\text{O}_2$	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A16,A17]	
$U_{\text{H}_2\text{O}_4 i,n,j,l}$	$\text{H}_2\text{PO}_4^-$ uptake by microbes	$\text{g P m}^{-2} \text{ h}^{-1}$	[A26e,A29]	
$U_{\text{HO}_4 i,n,j,l}$	$\text{HPO}_4^{2-}$ uptake by microbes	$\text{g P m}^{-2} \text{ h}^{-1}$	[A26f,A29]	
$U'_{\text{PO}_4}$	maximum $U_{\text{PO}_4}$ at 25 °C and non-limiting $\text{H}_2\text{PO}_4^-$	$\text{g P m}^{-2} \text{ h}^{-1}$	[A26d,e,f]	$5.0 \times 10^{-3}$
$V_{i,l,C}$	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]	
$X_{Cmn}$	minimum C internal recycling fraction	-	[A23a]	0.167
$X_{Cmx}$	maximum C internal recycling fraction	-	[A23a]	0.333
$X_{N,P}$	maximum N,P internal recycling fraction	-	[A23b]	0.833
$Y_g$	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	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-Atmosphere 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-atmosphere system. The first stage of this solution requires convergence to a value of canopy surface temperature  $T_c$  for each living and dead plant population at which the first-order closure of the canopy energy balance [B1a], including net radiation  $R_n$  [B1b], surface latent heat flux  $LE_c$  [B1c,d], surface sensible heat flux  $H_s$  [B1f], and change in canopy heat storage ( $G$ ) is achieved. These fluxes are controlled by surface aerodynamic ( $r_{ac}$ ) [B3d] and canopy stomatal ( $r_{sc}$ ) [B2] resistances. Vapor concentrations and temperatures in the canopy air ( $e_q$  and  $T_q$ ) resulting from  $LE_c$  and  $H_c$  drive latent ( $LE_q$ ) [B1e] and sensible ( $H_q$ ) [B1g] heat exchange with the atmosphere (Fig. 1).

Two controlling mechanisms are postulated for  $r_{sc}$  which are solved in two successive steps:

- (1) At the leaf level, leaf resistance  $r_l$  [C4 in S3 below] controls gaseous  $CO_2$  diffusion through each leaf surface when calculating  $CO_2$  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  $r_{lmin}$  [C5] for each leaf surface that allows a set ratio for intercellular to canopy  $CO_2$  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 is allowed to vary with canopy water status as described in S3: *Gross Primary Productivity* below when  $\psi_c$  is solved in the second stage of the convergence solution, described under *Canopy Water Potential* below. Values of  $r_{lmin}$  are aggregated by leaf surface area to a canopy value  $r_{scmin}$  for use in the energy balance convergence scheme [B2a].
- (2) At the canopy level,  $r_{sc}$  rises from  $r_{scmin}$  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.

For canopy energy balance convergence solution see module 'CONVERGENCE SOLUTION FOR CANOPY ENERGY BALANCE AND WATER UPTAKE' in *nitro.f*

For vapor and heat exchange with the atmosphere see module 'CALCULATE CANOPY AIR TEMPERATURE, VAPOR CONCENTRATION' in *uptake.f*

For minimum canopy stomatal resistance see module 'MINIMUM CANOPY STOMATAL RESISTANCE' in *stomate.f*

For actual canopy resistance see module 'CANOPY STOMATAL RESISTANCE' in *uptake.f*

### *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 (S3 [C50]) (Grant, 1998) (Fig. 2).

For root water uptake see module 'ROOT WATER UPTAKE FROM SOIL-CANOPY WATER POTENTIALS' in uptake.f

For root and soil hydraulic resistances see module 'SOIL AND ROOT HYDRAULIC RESISTANCES TO ROOT WATER UPTAKE' in uptake.f

### *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.

For water potential convergence solution see module 'TEST TRANSPIRATION - ROOT WATER UPTAKE VS. CHANGE IN CANOPY WATER STORAGE' in uptake.f

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

### *Canopy Transpiration*

$Rn_{ci} + LE_{ci} + H_{ci} + G_{ci} = 0$	canopy energy balance	[B1a]
$Rn_{ci} = R_{Sci} + Rl_{Sci} - Rlu_{ci} - Rlc_{ci} + Rlg_{ci}$	canopy net radiation	[B1b]
$LE_{ci} = L (e_{q(T_{qi})} - e_{ci(T_{ci})}) / (r_{aci} + r_{ae})$	$LE$ from canopy air-surface evaporation	[B1c]
$LE_{ci} = L (e_{q(T_{ci})} - e_{ci(T_{ci}, \psi_{ci})}) / (r_{aci} + r_{sci})$	$LE$ from canopy air-surface transpiration	[B1d]
$LE_{qi} = L (e_a - e_{q(T_{qi})}) / r_{aqi}$	$LE$ from atmosphere-canopy air evapotranspiration	[B1e]
$H_{ci} = \rho C_p (T_{qi} - T_{ci}) / r_{aci}$	$H$ from canopy air-canopy surface sensible heat	[B1f]
$H_{qi} = \rho C_p (T_a - T_{qi}) / r_{aqi}$	$H$ from atmosphere-canopy air sensible heat	[B1g]
$r_{smini} = 0.64 (C_b - C_i') / V_c' i$	$r_{sc}$ driven by rates of carboxylation vs. diffusion	[B2a]
$r_{sci} = r_{smini} + (r_{smax} - r_{smini}) e^{(-\beta \psi_{ti})}$	$r_{sc}$ constrained by canopy turgor	[B2b]
$r_{aqi} = \{(\ln((z_u - z_{di}) / z_{ri})^2 / (K^2 u_a))\} / (1 - 10 Ri_{qi})$	$r_{aq}$ driven by windspeed, surface roughness, buoyancy	[B3a]
$r_{aci} = r_{ac} / (1 - 3.2 Ri_{ci})$	$r_{ac}$ includes surface aerodynamic resistance	[B3b]
$Ri_{qi} = \{g (z_u - z_{ri}) / (u_a^2 T_a)\} (T_a - T_{qi})$	buoyancy effects on $r_{aq}$	[B3c]
$Ri_{ci} = \{g (z_u - z_{ri}) / (u_a^2 T_{qi})\} (T_{qi} - T_{ci})$	buoyancy effects on $r_{ac}$	[B3d]
$\psi_{ti} = \psi_{ci} - \psi_{\pi i}$	canopy turgor from total and osmotic water potentials	[B4]

### *Root and Mycorrhizal Water Uptake*

$U_{wi} = \sum_l \sum_r U_{wi,r,l}$		[B5]
$U_{wi,r,l} = (\psi_{c'i} - \psi_{s'l}) / (\mathcal{Q}_{si,r,l} + \mathcal{Q}_{ri,r,l} + \sum_x \mathcal{Q}_{ai,r,l,x})$	$U_w$ along hydraulic gradient	[B6]
$\psi_{c'i} = \psi_{ci} + 0.01 z_{bi}$		[B7]
$\psi_{s'l} = \psi_{sl} - 0.01 z_l$		[B8]
$\mathcal{Q}_{si,r,l} = \ln\{(d_{i,r,l} / r_{i,r,l}) / (2\pi L_{i,r,l} \kappa_{ri,r,l})\} \theta_{wl} / \theta_{pl}$		[B9]
$\mathcal{Q}_{ri,r,l} = \mathcal{Q}_{ri,r} / L_{i,r,l}$		[B10]
$\mathcal{Q}_{ai,r,l,x=1} = \mathcal{Q}_{ai,r} z_l / \{n_{i,r,l,1} (r_{i,r,l,1} / r'_{i,r})^4\} + \gamma \mathcal{Q}_{ai,r} z_{bi} / \{n_{i,r,l,1} (r_{bi} / r_{bi}')^4\}$		[B11]
$\mathcal{Q}_{ai,r,l,x=2} = \mathcal{Q}_{ai,r} (L_{i,r,l,2} / n_{i,r,l,2}) / \{n_{i,r,l,2} (r_{i,r,l,2} / r'_{i,r})^4\}$		[B12]
$\delta L_{i,r,l,1} / \delta t = \delta M_{i,r,l,1} / \delta t v_r / \{\rho_r (1 - \theta_{Pir}) (\pi r_{i,r,l,1}^2)\}$		[B13]



## Canopy Water Potential

$$\frac{(e_a - e_{i(T_{ci})}) / (r_{ai} + r_{ci})}{= \sum_l \sum_r (\psi_{ci}' - \psi_{si}') / (\Omega_{si,r,l} + \Omega_{ti,r,l} + \sum_x \Omega_{ai,r,l,x}) + X_{ci} \delta \psi_{ci} / \delta t}$$

$\psi_c$  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	Ref
<i>subscripts</i>					
<i>c</i>	canopy air				
<i>s</i>	canopy surface				
<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>r</i>	root or mycorrhizae				
<i>variables</i>					
$\beta$	stomatal resistance shape parameter	MPa <sup>-1</sup>	[B2b,C4,C9]	-5.0	Grant and Flanagan (2007)
<i>C<sub>b</sub></i>	[CO <sub>2</sub> ] in canopy air	μmol mol <sup>-1</sup>	[B2,C2,C5]		
<i>C<sub>i</sub>'<sub>i</sub></i>	[CO <sub>2</sub> ] in canopy leaves at $\psi_{ci} = 0$ MPa	μmol mol <sup>-1</sup>	[B2]	0.70 <i>C<sub>b</sub></i>	Larcher (2001)
<i>d<sub>i,r,l</sub></i>	half distance between adjacent roots	m	[B9]		
<i>E<sub>ci</sub></i>	canopy transpiration	m <sup>3</sup> m <sup>-2</sup> h <sup>-1</sup>	[B1,B14]		
<i>e<sub>a</sub></i>	atmospheric vapor density at <i>T<sub>a</sub></i> and ambient humidity	g m <sup>-3</sup>	[B1c]		
<i>e<sub>ci(T<sub>si</sub>,ψ<sub>ci</sub>)</sub></i>	canopy surface vapor density at <i>T<sub>si</sub></i> and $\psi_{ci}$	g m <sup>-3</sup>	[B1c,B1d]		
<i>e<sub>qi(T<sub>qi</sub>)</sub></i>	canopy air vapor density at <i>T<sub>qi</sub></i>	g m <sup>-3</sup>	[B1c,B1d,B1e]		
<i>G<sub>ci</sub></i>	canopy storage heat flux	W m <sup>-2</sup>	[B1a]		
<i>H<sub>ci</sub></i>	sensible heat flux from canopy air canopy surface	W m <sup>-2</sup>	[B1f]		
<i>H<sub>qi</sub></i>	sensible heat flux from atmodshere to canopy air	W m <sup>-2</sup>	[B1g]		
<i>K</i>	von Karman's constant		[B3a]	0.41	
<i>κ<sub>ti,r,l</sub></i>	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	MJ Mg <sup>-1</sup>	[B1c,B1d,B1e]	2460	
$LE_{ci}$	latent heat flux between canopy air and canopy surface	W m <sup>-2</sup>	[B1c,B1d]		
$LE_{qi}$	latent heat flux between atmosphere and canopy	W m <sup>-2</sup>	[B1e]		
$M_{i,r,l}$	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]		
$\mathcal{R}_{ai,r}$	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)
$\mathcal{R}_{ai,r,l,x}$	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]		
$\mathcal{R}_{ri,r}$	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)
$\mathcal{R}_{ri,r,l}$	radial resistance to water transport from surface to axis of roots or mycorrhizae	MPa h m <sup>-1</sup>	[B6,B10]		
$\mathcal{R}_{si,r,l}$	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]		
$\theta_{pi,r}$	root porosity	m <sup>3</sup> m <sup>-3</sup>	[B13]		
$Ri_{qi}$	Richardson number for atmosphere-canopy air heat exchange		[B3a,B3c]		van Bavel and Hillel (1976)
$Ri_{ci}$	Richardson number for canopy air-canopy surface heat exchange		[B3b,B3d]		
$Rlc_{ci}$	canopy-ground longwave radiation	W m <sup>-2</sup>	[B1b]		
$Rlg_{ci}$	ground-canopy longwave radiation	W m <sup>-2</sup>	[B1b]		
$Rls_{ci}$	sky-canopy longwave radiation	W m <sup>-2</sup>	[B1b]		
$Rlu_{ci}$	canopy-sky longwave radiation	W m <sup>-2</sup>	[B1b]		
$Rn_{ci}$	canopy net radiation	W m <sup>-2</sup>	[B1a,B1b]		
$RS_{ci}$	canopy shortwave radiation	W m <sup>-2</sup>	[B1b]		
$r_{ac}$	isothermal aeodynamic resistance to heat transfer at canopy surfaces	s m <sup>-1</sup>	[B3b]	10	
$r_{ae}$	surface resistance to free water evaporation	s m <sup>-1</sup>	[B1c]	50	
$r_{aci}$	aerodynamic resistance from canopy air to canopy surface	s m <sup>-1</sup>	[B1c,B1d,B1f,B3b,B		
$r_{aqi}$	aerodynamic resistance to vapor flux from atmosphere to canopy air	s m <sup>-1</sup>	[B1e,B1g,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]		

$r_{sci}$	stomatal resistance to vapor flux at canopy surface	s m <sup>-1</sup>	[B1d,B2b]		
$r_{scmaxi}$	canopy cuticular resistance to vapor flux	s m <sup>-1</sup>	[B2b]	5.0 x 10 <sup>3</sup>	Larcher (2001)
$r_{scmini}$	minimum $r_{sci}$ at $\psi_{ci} = 0$ MPa	s m <sup>-1</sup>	[B2a,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 $\psi_{ri,l,z} = 0$ 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	
$r_s$	minimum surface aerodynamic resistance to heat flux	s m <sup>-1</sup>	[B3d]	5	
$\rho_r$	root specific density	g C g FW <sup>-1</sup>	[B13]	0.05	Grant (1998)
$T_a$	atmosphere air temperature	K	[B1g,B3c]		
$T_{ci}$	canopy surface temperature	K	[B1f,B3d]		
$T_{qi}$	canopy air temperature	K	[B1f,B1g,B3c,B3d]		
$U_{wi}$	total water uptake from all rooted soil layers	m <sup>3</sup> m <sup>-2</sup> h <sup>-1</sup>	[B5,B14]		
$U_{wi,r,l}$	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,B3c,B3d]		
$V_c' i$	potential canopy CO <sub>2</sub> fixation rate at $\psi_{ci} = 0$ 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]		
$\psi_{ni}$	canopy osmotic potential	MPa	[B4]		
$\psi_{sl}$	soil water potential	MPa	[B8]		
$\psi_s' l$	$\psi_{sl}$ + 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,B3c,B3d]		Perrier (1982)
$z_u$	height of wind speed measurement	m	[B3a,B3c,B3d]		

### **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 S2 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  $r_{\min}$  at zero  $\psi_c$  [C5] to  $r_c$  at ambient  $\psi_c$  [C4], and by non-stomatal effects  $f_{\psi}$  [C9] on  $\text{CO}_2$ - 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  $\text{CO}_2$  fixation rate at convergence is multiplied by the area of each leaf surface, defined by node, elevation, azimuth, inclination and exposure (sunlit or shaded), to arrive at a value for gross primary productivity ( $GPP$ ) by each plant population in the model [C1]. The  $\text{CO}_2$  fixation product is stored in nonstructural C pools  $\sigma_c$  in each branch.

$GPP$  is strongly controlled by nutrient uptake  $U_{\text{NH}_4}$ ,  $U_{\text{NO}_3}$  and  $U_{\text{PO}_4}$  [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 Litterfall* below. Low  $\sigma_N:\sigma_c$  or  $\sigma_P:\sigma_c$  in branches indicate excess  $\text{CO}_2$  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  $\text{CO}_2$  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  $\text{CO}_2$  fixation.

For  $GPP$  see module 'C3 PHOTOSYNTHESIS' in grosu.b.f

For nutrient effects on  $GPP$  see module 'FEEDBACK ON C3 CARBOXYLATION FROM NON-STRUCTURAL C:N:P' in stomate.f

For nutrient effects on growth see module 'GROWTH RESPIRATION MAY BE LIMITED BY NON-STRUCTURAL N,P' in grosu.b.f

#### *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  $\text{O}_2$  uptake  $U_{\text{O}_2}$  [C14b] calculated by solving for aqueous  $\text{O}_2$  concentrations at root and mycorrhizal surfaces [ $\text{O}_{2r}$ ] at which convection + radial diffusion through the soil aqueous phase plus radial diffusion through the root aqueous phase [C14d] equals active uptake driven by  $\text{O}_2$  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  $\text{O}_2$  concentrations sustained by transport and dissolution of gaseous  $\text{O}_2$  through soil (S4 below) and roots (Grant 2004), and are governed by lengths and surface areas of roots and mycorrhizae (Grant, 1998). Thus  $R_c$  is coupled to  $\text{O}_2$  reduction by all root and mycorrhizal populations according to  $\text{O}_2$  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] with consequent litterfall of associated non-remobilizable C described below.

For oxidation of nonstructural C in shoot see module 'RESPIRATION FROM NON-STRUCTURAL C' in grosub.f

For oxidation of nonstructural C in root see module 'O2-UNLIMITED SECONDARY ROOT RESPIRATION FROM NON-STRUCTURAL C' in grosub.f

For root O<sub>2</sub> uptake see module 'SOLVE FOR GAS EXCHANGE IN SOIL AND ROOTS DURING ROOT UPTAKE' in uptake.f

### *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. Leaf, petiole and stalk growth drive leaf, petiole and internode extension and thus vertical leaf area profile and radiation interception. Root growth drives primary and secondary root extension and thus vertical root length and area profiles and thus root O<sub>2</sub> and nutrient uptake.

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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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  $\Omega_s$ ,  $\Omega_t$  and  $\Omega_a$ , and hence increase  $U$  [B6], thereby partly 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 and nutrients.

$R_s$  [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.

For shoot growth see module ‘C,N,P GROWTH OF LEAF, SHEATH OR PETIOLE, STALK ...’ in grosub.f

For root growth see module ‘TOTAL NON-STRUCTURAL C,N,P USED IN SECONDARY ROOT GROWTH’ in grosub.f

For shoot-root translocation see module ‘TRANSFER NON-STRUCTURAL C,N,P BETWEEN ROOT AND SHOOT’ in grosub.f

For senescence and litterfall see module ‘REMOBILIZATION AND LITTERFALL WHEN GROWTH RESPIRATION < 0 ...’ in grosub.f

For recycling during senescence see module ‘RECOVERY OF REMOBILIZABLE C,N,P ...’ in grosub.f

For exudation see module ‘ROOT EXUDATION OF C, N AND P ...’ in uptake.f

For shoot growth allocation see module ‘PARTITION GROWTH WITHIN EACH BRANCH FROM GROWTH STAGE’ in grosub.f

### *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  $[NH_4^+]$ ,  $[NO_3^-]$ ,  $[H_2PO_4^-]$  and  $[HPO_4^{2-}]$  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 [C23i]. Root N and P uptake is also constrained by root  $O_2$  uptake from  $O_2$  in soil and root aqueous phases [C14c,d,e] governed by  $O_2$  transfer in soil and root gaseous phases.

For root and mycorrhizal N and P uptake see module ‘NUTRIENT UPTAKE’ in uptake.f

For root and mycorrhizal  $O_2$  uptake see module ‘SOLVE FOR GAS EXCHANGE IN SOIL AND ROOTS DURING ROOT UPTAKE’ in uptake.f

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

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

In  $C_4$  plants, the mesophyll carboxylation rate is the lesser of  $CO_2$ - and light-limited reaction rates [C26] (Berry and Farquhar, 1978). The  $CO_2$ -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.

For C<sub>4</sub> carboxylation see module 'C<sub>4</sub> CARBOXYLATION REACTIONS IN MESOPHYLL' in grosub.f

#### *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 (Laik 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> (Laik 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).

For C<sub>4</sub> exchange see module 'MESOPHYLL TO BUNDLE SHEATH TRANSFER' in grosub.f

#### *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.

For C<sub>4</sub> bundle sheath carboxylation see module 'C3 CARBOXYLATION REACTIONS IN BUNDLE SHEATH OF C4 PLANTS' in grosub.f

For C<sub>4</sub> bundle sheath decarboxylation see module 'BUNDLE SHEATH CO<sub>2</sub> DECARBOXYLATION' in grosub.f

### *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  $Z_{rN,P}$ .

For shoot-root transfer see module 'TRANSFER NON-STRUCTURAL C,N,P BETWEEN ROOT AND SHOOT' in grosub.f

For root-mycorrhizal transfer see module 'TRANSFER NON-STRUCTURAL C,N,P BETWEEN ROOT AND MYCORRHIZAE ...' in grosub.f



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

<i>C<sub>3</sub> Gross Primary Productivity</i>	
$GPP = \sum_{i,j,k,l,m,n,o} (V_{ci,j,k,l,m,n,o} - V_{gi,j,k,l,m,n,o}) A_{i,j,k,l,m,n,o} CF_i$	solve for $C_{ii,j,k,l,m,n,o}$ at which
$V_{gi,j,k,l,m,n,o} = (C_b - C_{ii,j,k,l,m,n,o}) / r_{li,j,k,l,m,n,o}$	$V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}$
$V_{ci,j,k,l,m,n,o} = \min\{V_{bi,j,k,l,m,n,o}, V_{ji,j,k,l,m,n,o}\}$	diffusion
$r_{li,j,k,l,m,n,o} = r_{mini,j,k,l,m,n,o} + (r_{lmaxi} - r_{mini,j,k,l,m,n,o}) e^{(-\beta \psi_{ti})}$	carboxylation
$r_{mini,j,k,l,m,n,o} = (C_b - C_i) / V_{ci,j,k,l,m,n,o}$	$r_l$ is leaf-level equivalent of $r_c$
$V_{bi,j,k,l,m,n,o} = V_{bmax,i,j,k} (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (C_{ci,j,k,l,m,n,o} + K_{ci}) f_{\psi_{i,j,k,l,m,n,o}}$	minimum $r_l$ is driven by carboxylation
$V_{bmax,i,j,k} = V_{b'} F_{rubisco_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{tbi} f_{ci}$	CO <sub>2</sub> and water $f_{\psi}$ constraints on $V_b$ temperature $f_{tb}$ and nutrient $f_{ic}$ constraints on $V_{bmax}$
$\Gamma_{i,j,k} = 0.5 O_c V_{omax,i,j,k} K_{ci} / (V_{bmax,i,j,k} K_{oi})$	CO <sub>2</sub> compensation point
$V_{omax,i,j,k} = V_{o'} F_{rubisco_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{toi}$	oxygenation
$K_{ci} = K_{ci} f_{tkci} (1 + O_c / (K_{oi} f_{tkoi}))$	M-M constant for $V_b$
$V_{ji,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o} Y_{i,j,k,l,m,n,o} f_{\psi_{i,j,k,l,m,n,o}}$	
$Y_{i,j,k,l,m,n,o} = (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (4.5 C_{ci,j,k,l,m,n,o} + 10.5 \Gamma_{i,j,k})$	water constraints on $V_j$
$J_{i,j,k,l,m,n,o} = (\epsilon I_{i,l,m,n,o} + J_{max,i,j,k} - ((\epsilon I_{i,l,m,n,o} + J_{max,i,j,k})^2 - 4\alpha\epsilon I_{i,l,m,n,o} J_{max,i,j,k})^{0.5}) / (2\alpha)$	carboxylation efficiency of $V_j$
$J_{max,i,j,k} = V_{j'} F_{chlorophyll_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{tji} f_{ci}$	irradiance constraints on $J$
$f_{\psi_{i,j,k,l,m,n,o}} = (r_{min,i,j,k,l,m,n,o} / r_{i,j,k,l,m,n,o})^{0.5}$	temperature and nutrient constraints on $J_{max}$
$f_{tbi} = \exp[B_v - H_{av} / (RT_{ci})] / \{1 + \exp[(H_{al} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - H_{ah}) / (RT_{ci})]\}$	non-stomatal effect related to stomatal effect
$f_{toi} = \exp[B_o - H_{ao} / (RT_{ci})] / \{1 + \exp[(H_{al} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - H_{ah}) / (RT_{ci})]\}$	Arrhenius functions for carboxylation, oxygenation and electron transport
$f_{tji} = \exp[B_j - H_{aj} / (RT_{ci})] / \{1 + \exp[(H_{al} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - H_{ah}) / (RT_{ci})]\}$	temperature sensitivity of $K_{ci}$
$f_{tkci} = \exp[B_{kc} - H_{akc} / (RT_{ci})]$	temperature sensitivity of $K_{oi}$
$f_{tkoi} = \exp[B_{ko} - H_{ako} / (RT_{ci})]$	
$f_{ci} = \min\{\sigma_{Ni,j} / (\sigma_{Ni,j} + \sigma_{Ci,j} / K_{iCN}), \sigma_{Pi,j} / (\sigma_{Pi,j} + \sigma_{Ci,j} / K_{iCP})\}$	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

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

growth of remobilizable leaf protein C [C12]

### *Autotrophic Respiration*

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

total autotrophic respiration [C13]

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

shoot autotrophic respiration [C14a]

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

O<sub>2</sub> constraint on root respiration from active [C14b]

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

uptake coupled with [C14c]

$$= U_{w_{i,r,l}} [\text{O}_{2\text{sl}}] + 2\pi L_{i,r,l} D_{\text{SO}_2} ([\text{O}_{2\text{sl}}] - [\text{O}_{2\text{ri,r,l}}]) \ln\{(r_{\text{sl}} + r_{\text{ri,r,l}}) / r_{\text{ri,r,l}}\} + 2\pi L_{i,r,l} D_{\text{rO}_2} ([\text{O}_{2\text{qi,r,l}}] - [\text{O}_{2\text{ri,r,l}}]) \ln(r_{\text{qi,r,l}} / r_{\text{ri,r,l}})$$

diffusion of O<sub>2</sub> from soil and from active uptake coupled with diffusion of O<sub>2</sub> from roots [C14d]

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

[C14e]

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

remobilization in branches, roots and mycorrhizae [C15]

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

when  $R_m > R_c$

$$R_{\text{mi},j} = \sum_z (N_{i,j,z} R_m' f_{\text{tmi}})$$

maintenance respiration of branches, roots and [C16]

$$R_{\text{mi},r,l} = \sum_z (N_{i,r,l,z} R_m' f_{\text{tmi}})$$

mycorrhizae

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

growth respiration of branches, roots and [C17]

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

mycorrhizae when  $R_m < R_c$

### *Growth and Litterfall*

$$l_{i,j,zC} = R_{si,j} M_{L_N i,j} / M_{L_R i,j} (1.0 - (X_{Cmn} + (X_{Cmx} - X_{Cmn}) f_{\lambda Ci,j}))$$

senescence drives litterfall of non- remobilizable C [C18a]

$$l_{i,j,zN} = l_{i,j,zC} N_{\text{prot}} (1.0 - X_N f_{\lambda Ni,j})$$

less C recycling [C18b]

$$l_{i,j,zP} = l_{i,j,zC} P_{\text{prot}} (1.0 - X_P f_{\lambda Pi,j})$$

litterfall of N and P is driven by that of C less N and P [C18c]

$$f_{\lambda Ci,j} = \min\{\sigma_{Ni,j} / (\sigma_{Ni,j} + \sigma_{Ci,j} K_{\lambda N}), \sigma_{Pi,j} / (\sigma_{Pi,j} + \sigma_{Ci,j} K_{\lambda P})\}$$

recycling root and mycorrhizal litterfall calculated as for litterfall [C19a]

$$f_{\lambda Ni,j} = \sigma_{Ci,j} / (\sigma_{Ci,j} + \sigma_{Ni,j} / K_{\lambda N})$$

C, N and P recycling calculated [C19b]

$$f_{\lambda Pi,j} = \sigma_{Ci,j} / (\sigma_{Ci,j} + \sigma_{Pi,j} / K_{\lambda P})$$

from nonstructural C,N,P ratios [C19c]

$$x_{i,r,lC} = r_x \sigma_{Ci,r,l}$$

root and mycorrhizal exudation driven by  $\sigma_C$ ,  $\sigma_N$  [C19d]

$$x_{i,r,lN} = r_x \sigma_{Ni,r,l} f_{xi,r,lN}$$

and  $\sigma_P$ , and by  $\sigma_C$ :  $\sigma_N$  [C19e]

$$x_{i,r,lP} = r_x \sigma_{Pi,r,l} f_{xi,r,lP}$$

$\sigma_C$ :  $\sigma_P$ . [C19f]

$$f_{xi,r,lN} = \sigma_{Ni,j} / (\sigma_{Ni,j} + \sigma_{Ci,j} / K_{\lambda N})$$

[C19g]

$$f_{xi,r,lP} = \sigma_{Pi,j} / (\sigma_{Pi,j} + \sigma_{Ci,j} / K_{\lambda P})$$

[C19h]

$$\delta M_{Bi,j} / \delta t = \Sigma z [R_{gi,j} (1 - Y_{gi,z}) / Y_{gi,z}] - R_{si,j} - l_{i,j,C} \quad \text{branch growth driven by } R_g \quad [C20a]$$

$$\delta M_{Ri,r,l} / \delta t = [R_{gi,r,l} (1 - Y_{gi,r}) / Y_{gi,r}] - R_{si,r,l} - l_{i,r,l,C} \quad \text{root growth driven by } R_g \quad [C20b]$$

$$\delta A_{Li,j,k,l} / \delta t = \chi (M_{Li,j,k,l} / y_i)^{-0.33} \delta M_{Li,j,k,l} / \delta t \min\{1, \max\{0, \psi_{ti} - \psi_{ti}'\}\} \quad \text{leaf expansion driven by leaf mass growth} \quad [C21a]$$

$$\delta L_{i,r,l,l} / \delta t = (\delta M_{Ri,r,l,l} / \delta t) / y_i v_r / \{\rho_r (1 - \theta_{P_{i,r}}) (\pi r_{ti,r,l}^2)\} \quad \text{root extension of primary and secondary axes driven by root mass growth} \quad [C21b]$$

$$\delta L_{i,r,l,2} / \delta t = (\delta M_{Ri,r,l,2} / \delta t) v_r / \{\rho_r (1 - \theta_{P_{i,r}}) (\pi r_{ti,r,l,2}^2)\} \quad [C21c]$$

$$f_{tai} = T_{ci} \{ \exp[B_a - H_{aa} / (RT_{ci})] / \{1 + \exp[(H_{dl} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - H_{dh}) / (RT_{ci})]\} \} \quad \text{Arrhenius function for } R_a \quad [C22a]$$

$$f_{tmi} = T_{ci} \{ \exp[B_m - H_{aa} / (RT_{ci})] / \{1 + \exp[(H_{dl} - ST_{ci}) / (RT_{ci})]\} \} \quad \text{Arrhenius function for } R_m \quad [C22b]$$

### Root and Mycorrhizal Nutrient Uptake

$$U_{NH4i,r,l} = \{ U_{wi,r,l} [NH_4^+] + 2\pi L_{i,r,l} D_{eNH4l} ([NH_4^+] - [NH_4^+_{i,r,l}] / \ln(d_{i,r,l} / r_{ti,r,l})) \} \quad \text{root N and P uptake from mass flow} \quad [C23a]$$

$$= U'_{NH4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NH_4^+_{i,r,l}] - [NH_4^{+mn}]) / ([NH_4^+_{i,r,l}] - [NH_4^{+mn}] + K_{NH4}) f_{tai,l} f_{iNi,r,l} \quad \text{+ diffusion coupled with active uptake of } NH_4^+, NO_3^-, H_2PO_4^- \quad [C23b]$$

$$U_{NO3i,r,l} = \{ U_{wi,r,l} [NO_3^-] + 2\pi L_{i,r,l} D_{eNO3l} ([NO_3^-] - [NO_3^-_{i,r,l}] / \ln(d_{i,r,l} / r_{ti,r,l})) \} \quad \text{and } HPO_4^{2-} \text{ constrained by } O_2 \text{ uptake,} \quad [C23c]$$

$$= U'_{NO3} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NO_3^-_{i,r,l}] - [NO_3^{-mn}]) / ([NO_3^-_{i,r,l}] - [NO_3^{-mn}] + K_{NO3}) f_{tai,l} f_{iNi,r,l} \quad \text{as modelled for microbial N and P uptake in [A26]} \quad [C23d]$$

$$U_{H2PO4i,r,l} = \{ U_{wi,r,l} [H_2PO_4^-] + 2\pi L_{i,r,l} D_{ePO4l} ([H_2PO_4^-] - [H_2PO_4^-_{i,r,l}] / \ln(d_{i,r,l} / r_{ti,r,l})) \} \\ = U'_{PO4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([H_2PO_4^-_{i,r,l}] - [H_2PO_4^{-mn}]) / ([H_2PO_4^-_{i,r,l}] - [H_2PO_4^{-mn}] + K_{PO4}) f_{tai,l} f_{iPi,r,l} \quad [C23g]$$

$$U_{HPO4i,r,l} = \{ U_{wi,r,l} [HPO_4^{2-}] + 2\pi L_{i,r,l} D_{ePO4l} ([HPO_4^{2-}] - [HPO_4^{2-}_{i,r,l}] / \ln(d_{i,r,l} / r_{ti,r,l})) \} \\ = U'_{PO4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([HPO_4^{2-}_{i,r,l}] - [HPO_4^{2-mn}]) / ([HPO_4^{2-}_{i,r,l}] - [HPO_4^{2-mn}] + K_{PO4}) f_{tai,l} f_{iPi,r,l} \quad [C23i]$$

$$f_{iNi,r,l} = \sigma_{Ci,r,l} / (\sigma_{Ci,r,l} + \sigma_{Ni,r,l} / K_{iNC}) \quad \text{product inhibition of } U_{NH4}, U_{NO3} \text{ and } U_{PO4} \text{ determined by } \sigma_N \text{ and } \sigma_P \text{ vs. } \sigma_C \text{ in roots} \quad [C23j]$$

$$f_{iPi,r,l} = \sigma_{Ci,r,l} / (\sigma_{Ci,r,l} + \sigma_{Pi,r,l} / K_{iPC})$$

### C4 Gross Primary Productivity

#### C4 Mesophyll

$$GPP = \Sigma_{i,j,k,l,m,n,o} (V_{g(m4)ij,k,l,m,n,o} - V_{c(m4)ij,k,l,m,n,o}) \quad [C24]$$

$$V_{g(m4)ij,k,l,m,n,o} = (C_b - C_{i(m4)ij,k,l,m,n,o}) / r_{fi,j,k,l,m,n,o} \quad \text{gaseous diffusion} \quad [C25]$$

$$V_{c(m4)ij,k,l,m,n,o} = \min\{V_{b(m4)ij,k,l,m,n,o}, V_{j(m4)ij,k,l,m,n,o}\} \quad \text{mesophyll carboxylation} \quad [C26]$$

$$r_{fi,j,k,l,m,n,o} = r_{fmini,j,k,l,m,n,o} + (r_{lfmaxi} - r_{fmini,j,k,l,m,n,o}) e^{(-\beta \psi_{ti})} \quad [C27]$$

$$r_{fmini,j,k,l,m,n,o} = (C_b - C_{i(m4)'i}) / V_{c0(m4)ij,k,l,m,n,o} \quad [C28]$$

$$V_{b(m4)ij,k,l,m,n,o} = V_{bmax(m4)ij,k} (C_{c(m4)ij,k,l,m,n,o} - \Gamma_{(m4)ij,k}) / (C_{c(m4)ij,k,l,m,n,o} + K_{c(m4)i}) \quad \text{CO}_2\text{-limited carboxylation} \quad [C29]$$

$V_{j(m4)i,j,k,l,m,n,o} = J_{(m4)i,j,k,l,m,n,o} Y_{(m4)i,j,k,l,m,n,o}$	light-limited carboxylation	[C30a]
$Y_{(m4)i,j,k} = (C_{c(m4)i,j,k,l,m,n,o} - \Gamma_{(m4)i,j,k}) / (3.0 C_{c(m4)i,j,k,l,m,n,o} + 10.5 \Gamma_{(m4)i,j,k})$	carboxylation efficiency of $V_{j(m4)}$	[C30b]
$J_{(m4)i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\max(m4)i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\max(m4)i,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\max(m4)i,j,k})^{1/2})$	irradiance response function	[C31]
$V_{b\max(m4)i,j,k} = V_{b\max(m4)}' [N_{\text{pep}(m4)i,j,k}]' N_{\text{lf}i,j,k} A_{\text{lf}i,j,k} f_{C(m4)i,j,k} f_{\psi i} f_{\text{tvi}}$	PEPc activity	[C32]
$J_{\max(m4)i,j,k} = J_{\max}' [N_{\text{chl}(m4)i,j,k}]' N_{\text{lf}i,j,k} A_{\text{lf}i,j,k} f_{C(m4)i,j,k} f_{\psi i} f_{\text{tvi}}$	chlorophyll activity	[C33]
$f_{C(m4)i,j,k} = 1.0 / (1.0 + [\chi_{C4(m4)i,j,k}] / K_{\text{I}\chi_{C4(m4)}})$	C4 product inhibition	[C34]
$f_{\psi i,j,k,l,m,n,o} = (r_{\text{fmin}i,j,k,l,m,n,o} / r_{\text{fi},i,j,k,l,m,n,o})^{0.5}$	non-stomatal water limitation	[C35]

#### *C<sub>4</sub> 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]
$V_{\chi C4(b4)i,j,k} = \kappa_{\chi C4(b4)} \chi_{C4(b4)i,j,k} / (1.0 + C_{c(b4)i,j,k} / K_{\text{I}\chi_{C4(b4)}})$	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]
$\delta \chi_{C4(m4)i,j,k} / \delta t = \Sigma_{l,m,n,o} V_{c(m4)i,j,k,l,m,n,o} - V_{\chi C4(m4)i,j,k}$	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]
$\delta C_{c(b4)i,j,k} / \delta t = V_{\chi C4(b4)i,j,k} - V_{\phi(b4)i,j,k} - \Sigma_{l,m,n,o} V_{c(b4)i,j,k,l,m,n,o}$	bundle sheath CO <sub>2</sub> concentration	[C42]

#### *C<sub>4</sub> 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]
$V_{b(b4)i,j,k} = V_{b\max(b4)i,j,k} (C_{c(b4)i,j,k} - \Gamma_{(b4)i,j,k}) / (C_{c(b4)i,j,k} + K_{c(b4)})$	CO <sub>2</sub> -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]
$J_{(b4)i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\max(b4)i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\max(b4)i,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\max(b4)i,j,k})^{0.5})$	irradiance response function	[C46]
$V_{b\max(b4)i,j,k} = V_{b\max(b4)}' [N_{\text{rub}(b4)i,j,k}]' N_{\text{lf}i,j,k} A_{\text{lf}i,j,k} f_{C(c3)i,j,k} f_{\psi i} f_{\text{tvi}}$	RuBPc activity	[C47]
$J_{\max(b4)i,j,k} = J_{\max}' [N_{\text{chl}(b4)i,j,k}]' N_{\text{lf}i,j,k} A_{\text{lf}i,j,k} f_{C(c3)i,j,k} f_{\psi i} f_{\text{tvi}}$	chlorophyll activity	[C48]
$f_{C(c3)i,j,k} = \min\{[\nu_{\text{lf}i,j}] / ([\nu_{\text{lf}i,j}] + [\chi_{c3(b4)i,j}] / K_{\text{I}\nu_{\text{lf}}}), [\pi_{\text{lf}i,j}] / ([\pi_{\text{lf}i,j}] + [\chi_{c3(b4)i,j}] / K_{\text{I}\pi_{\text{lf}}})\}$	C <sub>3</sub> product inhibition	[C49]

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

$Z_{sC_{i,j-i,r,l}} = g_{sC_{i,j-i,r,l}} (\sigma_{C_{i,j}} M_{\text{Ri},r,l} - \sigma_{C_{i,r,l}} M_{\text{Bi},j}) / (M_{\text{Ri},r,l} + M_{\text{Bi},j})$	shoot – root C transfer driven by $\sigma_C$ concentration gradients	[C50]
$Z_{sN_{\text{Pi},j-i,r,l}} = g_{sN_{\text{Pi},j-i,r,l}} (\sigma_{N_{\text{Pi},j}} \sigma_{C_{i,r,l}} - \sigma_{N_{\text{Pi},r,l}} \sigma_{C_{i,j}}) / (\sigma_{C_{i,r,l}} + \sigma_{C_{i,j}})$	shoot – root N,P transfer driven by $\sigma_{N,P}$ concentration gradients	[C51]
$Z_{rC_{i,j-i,r,l}} = g_{rC_{i,j-i,r,l}} (\sigma_{C_{i,r,l}} M_{\text{Mi},r,l} - \sigma_{C_{i,m,l}} M_{\text{Ri},r,l}) / (M_{\text{Mi},r,l} + M_{\text{Ri},r,l})$	root – mycorrhizal C transfer driven by $\sigma_C$ conc'n gradients	[C52]

$$Z_{rN,Pi,j-i,r,l} = g_{rN,Pi,j-i,r,l} \left( \sigma_{N,Pi,r,l} \sigma_{Ci,m,l} - \sigma_{N,Pi,m,l} \sigma_{Ci,r,l} \right) / \left( \sigma_{Ci,m,l} + \sigma_{Ci,r,l} \right)$$

root – mycorrhizal N,P transfer  
driven by  $\sigma_{N,P}$  conc'n gradients

[C53]

Definition of Variables in Table S3

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 vs. 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	MPa <sup>-1</sup>	[C4 C27,C35]	-5.0	Grant and Flanagan (2007)
<i>B<sub>a</sub></i>	parameter such that <i>f<sub>toi</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C22a]	25.229	
<i>B<sub>j</sub></i>	parameter such that <i>f<sub>tji</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C10c]	17.362	
<i>B<sub>kc</sub></i>	parameter such that <i>f<sub>tkci</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C10d]	16.136	
<i>B<sub>ko</sub></i>	parameter such that <i>f<sub>tkoi</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C10e]	8.067	
<i>B<sub>m</sub></i>	parameter such that <i>f<sub>tmj</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C22b]	25.216	
<i>B<sub>o</sub></i>	parameter such that <i>f<sub>toi</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C10b]	24.220	
<i>B<sub>v</sub></i>	parameter such that <i>f<sub>tvi</sub></i> = 1.0 at <i>T<sub>c</sub></i> = 298.15 K		[C10a]	26.237	
<i>C<sub>b</sub></i>	[CO <sub>2</sub> ] in canopy air	μmol mol <sup>-1</sup>	[C2,C5 C25,C28]		
<i>C<sub>c</sub></i>	[CO <sub>2</sub> ] in canopy chloroplasts in equilibrium with <i>C<sub>ii,j,k,l,m,n,o</sub></i>	μM	[C6a,C7b]		
<i>C<sub>c(b4)</sub></i>	[CO <sub>2</sub> ] in C <sub>4</sub> bundle sheath	μM	[C38,C39,C42,C44 , C45b]		
<i>C<sub>c(m4)</sub></i>	[CO <sub>2</sub> ] in C <sub>4</sub> mesophyll in equilibrium with <i>C<sub>ii,j,k,l,m,n,o</sub></i>	μM	[C29,C30b,C39]		
		-	[C1]		He (2016)
<i>CF<sub>i</sub></i>	clumping factor			0.45 (needleleaf) 0.675 (broadleaf) 0.70 x <i>C<sub>b</sub></i>	
<i>C<sub>i</sub>'</i>	[CO <sub>2</sub> ] in canopy leaves when <i>ψ<sub>ci</sub></i> = 0	μmol mol <sup>-1</sup>	[C5]		Larcher (2001)

$C_i$	[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 <sub>b</sub>	
$C_{i(m4)}$	[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]		
$D_{e\text{ NH}_4l}$	effective dispersivity-diffusivity of NH <sub>4</sub> <sup>+</sup> during root uptake	m <sup>2</sup> h <sup>-1</sup>	[C23]		
$D_{e\text{ NO}_3l}$	effective dispersivity-diffusivity of NO <sub>3</sub> <sup>-</sup> during root uptake	m <sup>2</sup> h <sup>-1</sup>	[C23]		
$D_{e\text{ PO}_4l}$	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]		
$D_{rO_2}$	aqueous diffusivity of O <sub>2</sub> from root aerenchyma to root or mycorrhizal surfaces	m <sup>2</sup> h <sup>-1</sup>	[C14d]		
$D_{sO_2}$	aqueous diffusivity of O <sub>2</sub> from soil to root or mycorrhizal surfaces	m <sup>2</sup> h <sup>-1</sup>	[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 <sup>-1</sup> or P <sup>-1</sup>	[C13]	2.15	Veen (1981)
$f_{C(c3)}$	C <sub>3</sub> product inhibition of RuBP carboxylation activity in C <sub>4</sub> bundle sheath or C <sub>3</sub> mesophyll		[C47,C48,C49]		
$f_{C(m4)}$	C <sub>4</sub> product inhibition of PEP carboxylation activity in C <sub>4</sub> 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	–	[C23i]		
$f_{iP}$	P inhibition on root P uptake	–	[C23j]		
$f_{\lambda C}$	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,C22a,C23]		
$f_{tb}$	temperature effect on carboxylation	–	[C6b,C10a]		
$f_{ij}$	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]		
$f_{to}$	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. (2000)
$f_{\psi i}$	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	Grant (1998)
$g_{sN,P}$	rate constant for shoot-root N,P transfer	$h^{-1}$	[C51]	0.1	Grant (1998)
$g_{rC}$	rate constant for root-mycorrhizal C transfer	$h^{-1}$	[C52]	0.1	Grant (1998)
$g_{rN,P}$	rate constant for root-mycorrhizal N,P transfer	$h^{-1}$	[C53]	0.1	Grant (1998)
$H_{aj}$	energy of activation for autotrophic, maintenance respiration	$J\ mol^{-1}$	[C22a,b]	$62.5 \times 10^3$	
$H_{aj}$	energy of activation for electron transport	$J\ mol^{-1}$	[C10c]	$43 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{akc}$	parameter for temperature sensitivity of $K_{c_i}$	$J\ mol^{-1}$	[C10d]	$40 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{ako}$	parameter for temperature sensitivity of $K_{o_i}$	$J\ mol^{-1}$	[C10e]	$20 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{ao}$	energy of activation for oxygenation	$J\ mol^{-1}$	[C10b]	$60 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{av}$	energy of activation for carboxylation	$J\ mol^{-1}$	[C10a]	$65 \times 10^3$	Bernacchi et al. (2001,2003)
$H_{dh}$	energy of high temperature deactivation	$J\ mol^{-1}$	[C10, C22]	$222.5 \times 10^3$	
$H_{dl}$	energy of low temperature deactivation	$J\ mol^{-1}$	[C10, C22]	$197.5 \times 10^3$	
$[H_2PO_4^{-}]_{i,r,l}$	concentration of $H_2PO_4^{-}$ root or mycorrhizal surfaces	$g\ P\ m^{-3}$	[C23e]		
$[H_2PO_4^{-}]_{mn}$	concentration of $H_2PO_4^{-}$ at root or mycorrhizal surfaces below which $U_{H_2PO_4} = 0$	$g\ P\ m^{-3}$	[C23f]	0.002	Barber and Silberbush, 1984
$[HPO_4^{2-}]_{i,r,l}$	concentration of $HPO_4^{2-}$ root or mycorrhizal surfaces	$g\ P\ m^{-3}$	[C23g]		
$[HPO_4^{2-}]_{mn}$	concentration of $HPO_4^{2-}$ at root or mycorrhizal surfaces below which $U_{HPO_4} = 0$	$g\ P\ m^{-3}$	[C23h]	0.002	
$I$	irradiance	$\mu mol\ m^{-2}\ s^{-1}$	[C8a]		
$J$	electron transport rate in $C_3$ mesophyll	$\mu mol\ m^{-2}\ s^{-1}$	[C7a,C8a]		
$J_{(b4)}$	electron transport rate in $C_4$ bundle sheath	$\mu mol\ m^{-2}\ s^{-1}$	[C45a,C46]		
$J_{(m4)}$	electron transport rate in $C_4$ mesophyll	$\mu mol\ m^{-2}\ s^{-1}$	[C30a,C31]		
$J_{max}'$	specific electron transport rate at non-limiting $I$ and $25^{\circ}C$ when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu mol\ g^{-1}\ s^{-1}$	[C33,C48]	400	
$J_{max(b4)}$	electron transport rate in $C_4$ bundle sheath at non-limiting $I$	$\mu mol\ m^{-2}\ s^{-1}$	[C46,C48]		

$J_{\max(m4)}$	electron transport rate in C <sub>4</sub> 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 C <sub>4</sub> bundle sheath	$\mu\text{M}$	[C44]	30.0 at 25°C and zero O <sub>2</sub>	Lawlor (1993)
$K_{c(m4)}$	Michaelis-Menten constant for carboxylation in C <sub>4</sub> mesophyll	$\mu\text{M}$	[C29]	3.0 at 25°C	Lawlor (1993)
$K_c$	Michaelis-Menten constant for carboxylation at zero O <sub>2</sub>	$\mu\text{M}$	[C6c,C6e]	12.5 at 25 °C	Farquhar et al. (1980)
$K_c$	Michaelis-Menten constant for carboxylation at ambient O <sub>2</sub>	$\mu\text{M}$	[C6e]		
$K_{iC_N}$	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. $\sigma_P$	$\text{g C g P}^{-1}$	[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	$\mu\text{M}$	[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	$\mu\text{M}$	[C34]	$5 \times 10^6$	
$K_{I\nu_{If}}$	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 [ $\nu_{fi,j}$ ]	$\text{g C g N}^{-1}$	[C49]	100	
$K_{I\pi_{If}}$	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 [ $\pi_{fi,j}$ ]	$\text{g C g P}^{-1}$	[C49]	1000	
$K_{iN_C}$	inhibition constant for N uptake in roots from $\sigma_{Ci,j}$ vs. $\sigma_{Nj}$	$\text{g N g C}^{-1}$	[C23]	0.1	Grant (1998)
$K_{iP_C}$	inhibition constant for P uptake in roots from $\sigma_{Ci,j}$ vs. $\sigma_{Pi,j}$	$\text{g P g C}^{-1}$	[C23]	0.01	Grant (1998)
$K_{\lambda N}$	constant used to calculate remobilization of leaf or root C and N during senescence	$\text{g N g C}^{-1}$	[C19a,C19b]	0.1	
$K_{\lambda P}$	constant used to calculate remobilization of leaf or root C and P during senescence	$\text{g P g C}^{-1}$	[C19a,C19c]	0.01	
$K_{NH_4}$	M-M constant for NH <sub>4</sub> <sup>+</sup> uptake at root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[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	$\text{g N m}^{-3}$	[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	$\text{g P m}^{-3}$	[C23]	0.125	Barber and Silberbush, 1984
$K_{O_2}$	Michaelis-Menten constant for root or mycorrhizal O <sub>2</sub> uptake	$\text{g m}^{-3}$	[C14c]	0.32	Griffin (1972)
$K_o$	inhibition constant for O <sub>2</sub> in carboxylation	$\mu\text{M}$	[C6c,C6e]	500 at 25 °C	Farquhar et al. (1980)
$K_{xN}$	inhibition constant for exudation of root or mycorrhizal N	$\text{g C g N}^{-1}$	[C19g]	1.0	
$K_{xP}$	inhibition constant for exudation of root or mycorrhizal P	$\text{g C g P}^{-1}$	[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	$\text{g N m}^{-2} \text{ h}^{-1}$	[C18b]	
$l_P$	P litterfall from leaf or root	$\text{g P m}^{-2} \text{ h}^{-1}$	[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, C52]	
$M_{L_{iprot}}$	leaf protein phytomass calculated from leaf N, P contents	$\text{g C m}^{-2}$	[C6b,C6d,C8b]	
$N, P$	N or P content of organ $z$	$\text{g N or P m}^{-2}$	[C16, C19]	
$N_{\text{leaf}}$	maximum leaf structural N content	$\text{g N g C}^{-1}$	[C12]	0.10
$N'_{\text{leaf}}$	minimum leaf structural N content	$\text{g N g C}^{-1}$	[C12]	$0.33 \times N_{\text{leaf}}$
$N_{\text{lf}}$	total leaf N	$\text{g N m}^{-2} \text{ leaf}$	[C32,C33,C47, C48]	
$N_{\text{prot}}$	N content of protein remobilized from leaf or root	$\text{g N C}^{-1}$	[C12,C18b]	0.4
$[N_{\text{chl(b4)}}]'$	ratio of chlorophyll N in $C_4$ bundle sheath to total leaf N	$\text{g N g N}^{-1}$	[C48]	0.025
$[N_{\text{chl(m4)}}]'$	ratio of chlorophyll N in $C_4$ mesophyll to total leaf N	$\text{g N g N}^{-1}$	[C33]	0.025
$[NH_4^+_{i,r,l}]$	concentration of $NH_4^+$ at root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[C23]	
$[NH_4^+_{mn}]$	concentration of $NH_4^+$ at root or mycorrhizal surfaces below which $U_{NH_4} = 0$	$\text{g N m}^{-3}$	[C23]	0.0125 Barber and Silberbush, 1984
$[NO_3^-_{i,r,l}]$	concentration of $NH_4^+$ at root or mycorrhizal surfaces	$\text{g N m}^{-3}$	[C23]	
$[NO_3^-_{mn}]$	concentration of $NO_3^-$ at root or mycorrhizal surfaces below which $U_{NO_3} = 0$	$\text{g N m}^{-3}$	[C23]	0.03 Barber and Silberbush, 1984
$[N_{\text{pep(m4)}}]'$	ratio of PEP carboxylase N in $C_4$ mesophyll to total leaf N	$\text{g N g N}^{-1}$	[C32]	0.025
$[N_{\text{rub(b4)}}]'$	ratio of RuBP carboxylase N in $C_4$ bundle sheath to total leaf N	$\text{g N g N}^{-1}$	[C47]	0.025
$O_{2q}$	aqueous $O_2$ concentration in root or mycorrhizal aerenchyma	$\text{g m}^{-3}$	[C14c,d]	
$O_{2r}$	aqueous $O_2$ concentration at root or mycorrhizal surfaces	$\text{g m}^{-3}$	[C14c,d]	
$O_{2s}$	aqueous $O_2$ concentration in soil solution	$\text{g m}^{-3}$	[C14c,d]	
$O_c$	$[O_2]$ in canopy chloroplasts in equilibrium with $O_2$ in atm.	$\mu\text{M}$	[C6c,C6e]	
$P_{\text{leaf}}$	maximum leaf structural P content	$\text{g P g C}^{-1}$	[C12]	0.01
$P'_{\text{leaf}}$	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

$[\pi_f]$	concentration of nonstructural root P uptake product in leaf	g P g C <sup>-1</sup>	[C49]		
$\theta_P$	root or mycorrhizal porosity	m <sup>3</sup> m <sup>-3</sup>	[C21b]	0.1 - 0.5	
$R$	gas constant	J mol <sup>-1</sup> K <sup>-1</sup>	[C10, C22]	8.3143	
$R_a$	total autotrophic respiration	g C m <sup>-2</sup> h <sup>-1</sup>	[C13]		
$R_a'$	$R_a$ under nonlimiting O <sub>2</sub>	g C m <sup>-2</sup> h <sup>-1</sup>	[C14]		
$R_c'$	specific autotrophic respiration of $\sigma_{C_{i,j}}$ at $T_{ci} = 25$ °C	g C g C <sup>-1</sup> h <sup>-1</sup>	[C14]	0.015	
$R_c$	autotrophic respiration of $\sigma_{C_{i,j}}$ or $\sigma_{C_{i,r,l}}$	g C m <sup>-2</sup> h <sup>-1</sup>	[C13,C14,C17, C15]		
$R_g$	growth respiration	g C m <sup>-2</sup> h <sup>-1</sup>	[C17,C20]		
$r_{lf}$	leaf stomatal resistance	s m <sup>-1</sup>	[C25,C27,C39]		
$r_{lmaxi}$	leaf cuticular resistance	s m <sup>-1</sup>	[C27]		
$r_{lmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	s m <sup>-1</sup>	[C27,C28,C35]		
$r_{l,j,k,l,m,n,o}$	leaf stomatal resistance	s m <sup>-1</sup>	[C2,C4,C9]		
$r_{lmaxi}$	leaf cuticular resistance	s m <sup>-1</sup>	[C4]		
$r_{lmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	s m <sup>-1</sup>	[C4,C5,C9]		
$R_m'$	specific maintenance respiration of $\sigma_{C_{i,j}}$ at $T_{ci} = 25$ °C	g C g N <sup>-1</sup> h <sup>-1</sup>	[C16]	0.01	Barnes et al. (1998)
$R_{mi,j}$	above-ground maintenance respiration	g C m <sup>-2</sup> h <sup>-1</sup>	[C16,C17,C15]		
$r_{qi,r,l}$	radius of root aerenchyma	m	[C14d]		
$r_{ri,r,l}$	root or mycorrhizal radius	m	[C14d,C21b,c,C23a,c,e]	$1.0 \times 10^{-4}$ or $5.0 \times 10^{-6}$	
$R_{si,j}$	respiration from remobilization of leaf C	g C m <sup>-2</sup> h <sup>-1</sup>	[C13,C15,C18a, C20]		
$r_{sl}$	thickness of soil water films	m	[C14d]		
$r_x$	rate constant for root or mycorrhizal exudation	h <sup>-1</sup>	[C19d,e,f]	$0.75 \times 10^{-3}$	
$\rho_r$	dry matter content of root biomass	g g <sup>-1</sup>	[C21b]	0.125	
$S$	change in entropy	J mol <sup>-1</sup> K <sup>-1</sup>	[C10, C22]	710	Sharpe and DeMichelle
$\sigma_C$	nonstructural C product of CO <sub>2</sub> fixation	g C g C <sup>-1</sup>	[C11,C19,C23i,j,C50-53]		
$\sigma_N$	nonstructural N product of root uptake	g N g C <sup>-1</sup>	[C11,C19.C23i, C51,C53]		
$\sigma_P$	nonstructural P product of root uptake	g P g C <sup>-1</sup>	[C11,C19,C23j, C51,C53]		
$T_c$	canopy temperature	K	[C10, C22]		
$U_{H_2PO_4i,r,l}$	H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> uptake by roots or mycorrhizae	g P m <sup>-2</sup> h <sup>-1</sup>	[C23e,f]		
$U_{HPO_4i,r,l}$	HPO <sub>4</sub> <sup>2-</sup> uptake by roots or mycorrhizae	g P m <sup>-2</sup> h <sup>-1</sup>	[C23g,h]		

$U_{\text{NH}_4 i, r, l}$	$\text{NH}_4^+$ 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
$U_{\text{NO}_3 i, r, l}$	$\text{NO}_3^-$ 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
$U'_{\text{PO}_4}$	maximum $U_{\text{H}_2\text{PO}_4}, U_{\text{HPO}_4}$ at 25 °C and non-limiting $\text{H}_2\text{PO}_4^-$ , $\text{HPO}_4^{2-}$	$\text{g P m}^{-2} \text{ h}^{-1}$	[C23]	$5.0 \times 10^{-3}$	Barber and Silberbush 1984
$U_{\text{O}_2 i, r, l}$	$\text{O}_2$ uptake by roots and mycorrhizae under ambient $\text{O}_2$	$\text{g O m}^{-2} \text{ h}^{-1}$	[C14b,c,C23b,d,f]		
$U'_{\text{O}_2 i, l, r}$	$\text{O}_2$ 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]		
$V_{\phi(\text{b}4) i, j, k}$	$\text{CO}_2$ leakage from $\text{C}_4$ bundle sheath to $\text{C}_4$ mesophyll	$\text{g C m}^{-2} \text{ h}^{-1}$	[C39,C42]		
$V_{\text{b}}'$	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 $\psi_{\text{ci}} = 0$ 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 $\psi_{\text{ci}} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{ s}^{-1}$	[C32]	150	
$V_{\text{bmax}(\text{m}4) i, j, k}$	$\text{CO}_2$ -nonlimited carboxylation rate in $\text{C}_4$ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C29,C32]		
$V_{\text{bmax} i, j, k}$	leaf carboxylation rate at non-limiting $\text{CO}_2$ , $\psi_{\text{ci}}$ , $T_{\text{c}}$ and N,P	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C6a,C6b,C6c]		
$V_{\text{c}(\text{b}4) i, j, k, l, m, n, o}$	$\text{CO}_2$ fixation rate in $\text{C}_4$ bundle sheath	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C43]		
$V_{\text{c}(\text{m}4) i, j, k, l, m, n, o}$	$\text{CO}_2$ fixation rate in $\text{C}_4$ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C24,C26,C40,C41]		
$V_{\text{c}0(\text{m}4) i, j, k, l, m, n, o}$	$\text{CO}_2$ fixation rate in $\text{C}_4$ mesophyll when $\psi_{\text{ci}} = 0$ MPa	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C28]		
$V_{\text{ci}, j, k, l, m, n, o}$	leaf $\text{CO}_2$ fixation rate	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C1,C3]		
$V_{\text{c}}'_{i, j, k, l, m, n, o}$	leaf $\text{CO}_2$ fixation rate when $\psi_{\text{ci}} = 0$	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C5]		
$V_{\text{g}(\text{m}4) i, j, k, l, m, n, o}$	$\text{CO}_2$ diffusion rate into $\text{C}_4$ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[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)
$V_{omaxi,j,k}$	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]		
$V_{\lambda C4(b4)i,j,k}$	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]		
$V_{\lambda C4(m4)}$	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]		
[ $v_f$ ]	concentration of nonstructural root N uptake product in leaf	g N g C <sup>-1</sup>	[C49]		
$v_r$	specific volume of root biomass	m <sup>3</sup> g <sup>-1</sup>	[C21b]		
$W_{lf(b4)}$	C <sub>4</sub> bundle sheath water content	g m <sup>-2</sup>	[C37,C39]		
$W_{lf(m4)}$	C <sub>4</sub> mesophyll water content	g m <sup>-2</sup>	[C37]		
$X_{Cmn}$	minimum fraction of remobilizable C translocated out of leaf or root during senescence	-	[C18a]	0.167	Kimmins (2004)
$X_{Cmx}$	maximum fraction of remobilizable C translocated out of leaf or root during senescence	-	[C18a]	0.50	Kimmins (2004)
$X_{N,P}$	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	[C18b,C18c]	0.83	Kimmins (2004)
$x_{i,r,l,C}$	root and mycorrhizal C exudation	g C m <sup>-2</sup> h <sup>-1</sup>	[C19d]		
$x_{i,r,l,N}$	root and mycorrhizal C exudation	g N m <sup>-2</sup> h <sup>-1</sup>	[C19e]		
$x_{i,r,l,P}$	root and mycorrhizal C exudation	g P m <sup>-2</sup> h <sup>-1</sup>	[C19f]		
$Y$	carboxylation yield from electron transport in C <sub>3</sub> mesophyll	μmol CO <sub>2</sub> μmol e <sup>-</sup> <sup>-1</sup>	[C7a,b]		
$Y_{(b4)}$	carboxylation yield from electron transport in C <sub>4</sub> bundle sheath	μmol CO <sub>2</sub> μmol e <sup>-</sup> <sup>-1</sup>	[C45a,b]		
$Y_{(m4)}$	carboxylation yield from electron transport in C <sub>4</sub> mesophyll	μmol CO <sub>2</sub> μmol e <sup>-</sup> <sup>-1</sup>	[C30a,b]		

$Y_g$	fraction of $\sigma_{C_{ij}}$ used for growth expended as $R_{gij,z}$ by organ $z$	$\text{g C g C}^{-1}$	[C20]	0.28 ( $z$ = leaf), 0.24 ( $z$ = root and other non-foliar), 0.20 ( $z$ = 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]		
$\Gamma$	CO <sub>2</sub> compensation point in C <sub>3</sub> mesophyll	$\mu\text{M}$	[C6a,C6c,C7b]		
$\Gamma_{(b4)}$	CO <sub>2</sub> compensation point in C <sub>4</sub> bundle sheath	$\mu\text{M}$	[C44,C45b]		
$\Gamma_{(m4)}$	CO <sub>2</sub> compensation point in C <sub>4</sub> mesophyll	$\mu\text{M}$	[C29,C30b]		
$\alpha$	shape parameter for response of $J$ to $I$ C <sub>3</sub>	-	[C8a]	0.7	
$\alpha$	shape parameter for response of $J$ to $I$ C <sub>4</sub>	-	[C31,C46]	0.75	
$\chi$	area:mass ratio of leaf growth	$\text{m g}^{-3}$	[C21]	0.0125	Grant and Hesketh (1992)
$\chi_{C4(b4)}$	non-structural C <sub>4</sub> fixation product in C <sub>4</sub> bundle sheath	$\text{g C m}^{-2}$	[C37,C38,C41]		
$\chi_{C4(m4)}$	non-structural C <sub>4</sub> fixation product in C <sub>4</sub> mesophyll	$\text{g C m}^{-2}$	[C37,C40]		
$[\chi_{c3(b4)}]$	concentration of non-structural C <sub>3</sub> fixation product in C <sub>4</sub> bundle sheath	$\text{g g}^{-1}$	[C49]		
$[\chi_{C4(m4)}]$	concentration of non-structural C <sub>4</sub> fixation product in C <sub>4</sub> mesophyll	$\mu\text{M}$	[C34]		
$\varepsilon$	quantum yield C <sub>3</sub>	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[C8a]	0.45	Farquhar et al. (1980)
$\varepsilon$	quantum yield C <sub>4</sub>	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[C31,C46]	0.45	Farquhar et al., (1980)
$\kappa_{Cc(b4)}$	conductance to CO <sub>2</sub> leakage from C <sub>4</sub> bundle sheath	$\text{h}^{-1}$	[C39]	20	
$\psi_c$	canopy turgor potential	MPa	[C4]	1.25 at $\psi_c = 0$	

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

### *Surface Water Flux*

Surface runoff downslope [D1a] is modelled from Manning's equation with surface water velocity  $v$  [D3] and mobile ponded water depth  $d_m$  [D2] calculated from surface water balance [D4] using kinematic wave theory. Runoff downslope is partitioned into east-west  $x$  and north-south  $y$  directions for transfers with adjacent grid cells [D1a] according to their relative slopes [D6]. Downslope snow transfer is modelled from windspeeds and partitioned into east-west  $x$  and north-south  $y$  directions for transfers with adjacent grid cells [D1b] such that over time these surfaces approach a common surface elevation across a landscape.

For runoff see module 'SURFACE WATER FLUX' in watsub.f

### *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 Poiseuille-Hagen theory for laminar flow in tubes (Dimitrov et al., 2010), depending on inputs for macropore volume fraction.

For micropore water flow see module 'WATER FLUX FROM WATER POTENTIALS, HYDRAULIC CONDUCTIVITY ...' in watsub.f

For macropore water flow see module 'MACROPORE FLOW FROM POISEUILLE FLOW ...' in watsub.f

### *Exchange with Water Table*

If a water table is present in the model, subsurface boundary water discharge or recharge between saturated boundary grid cells and a fixed external water table are calculated from lateral hydraulic conductivities of the grid cells, and from gravitational potential 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. Separate values of  $d_t$  and  $L_t$  can be set for artificial drainage from which only discharge can occur.

For micropore discharge to natural water table see module 'MICROPORE DISCHARGE ABOVE WATER TABLE' in watsub.f

For macropore discharge to natural water table see module 'MACROPORE DISCHARGE ABOVE WATER TABLE' in watsub.f

For micropore discharge to artificial water table see module 'MICROPORE DISCHARGE ABOVE TILE DRAIN' in watsub.f

For macropore discharge to artificial water table see module 'MACROPORE DISCHARGE ABOVE TILE DRAIN' in watsub.f

For micropore recharge from natural water table see module 'MICROPORE RECHARGE BELOW WATER TABLE' in watsub.f

For macropore recharge from natural water table see module 'MACROPORE RECHARGE BELOW WATER TABLE' in watsub.f

### *Surface Heat Flux*

Surface heat fluxes ( $G_s$ ) from closure of the energy balance at snowpack, surface litter and soil surfaces [D11a] (Grant et al., 1999) drive latent and sensible heat transfer ( $LE_s$  and  $H_s$ ) with air above the ground surface [D11d,D11f]. These transfers generate vapor concentrations and temperatures that drive latent ( $LE_q$ ) [D11c] and sensible ( $H_q$ ) [D11e] heat exchange between the air above the ground surface and the atmosphere.

For snowpack surface energy balance see module ‘HEAT AND VAPOR FLUXES BETWEEN SNOWPACK AND GROUND AIR’ in watsub.f

For litter surface energy balance see module ‘HEAT AND VAPOR FLUXES BETWEEN LITTER AND GROUND AIR’ in watsub.f

For soil surface energy balance see module ‘HEAT AND VAPOR FLUXES BETWEEN SOIL SURFACE AND GROUND AIR’ in watsub.f

For ground air-atmosphere vapor and heat exchange see module ‘AERODYNAMIC ENERGY EXCHANGE BETWEEN GROUND SURFACE AIR AND ATMOSPHERE’ in watsub.f

### *Subsurface Heat Flux*

Surface heat fluxes  $G_s$  drive conductive – convective fluxes  $G$  among snowpack layers, surface litter and soil layers [D12]. These fluxes drive freezing – thawing ( $Q_f$ ) and temperatures ( $T$ ) in snowpack layers, surface litter and soil layers [D13].

For freeze-thaw in snowpack layers see module ‘FREEZE-THAW IN SNOWPACK LAYER ...’ in watsub.f

For freeze-thaw in surface litter see module ‘FREEZE-THAW IN SURFACE LITTER ...’ in watsub.f

For freeze-thaw in soil micropore layers see module ‘FREEZE-THAW IN SOIL LAYER MICROPORE ...’ in watsub.f

For freeze-thaw in soil macropore layers see module ‘FREEZE-THAW IN SOIL LAYER MACROPORE ...’ in watsub.f

### *Gas Flux*

All gases undergo volatilization – dissolution between the gaseous and aqueous phases in the surface litter, soil [D14a] and root layers [D14b], and between the atmosphere and the aqueous phase at litter and soil surfaces [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].

For gas transfer in soil see module ‘GASEOUS TRANSPORT FROM GASEOUS DIFFUSIVITY AND CONCENTRATION ...’ in trnsfr.f

For gas transfer in roots see module ‘GAS TRANSFER THROUGH ROOTS’ in uptake.f

For volatilization – dissolution in soil see module ‘VOLATILIZATION-DISSOLUTION OF GASES IN SOIL ...’ in trnsfr.f

For volatilization – dissolution in roots see module ‘VOLATILIZATION-DISSOLUTION BETWEEN GASEOUS AND AQUEOUS PHASES IN ROOTS...’ in uptake.f

For bubbling see module ‘BUBBLING IF THE SUM OF ALL GASEOUS EQUIVALENT ...’ in trnsfr.f

### *Solute Flux*

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

For micropore solute transfer see module ‘SOLUTE TRANSPORT IN MICROPORES’ in trnsfr.f

For macropore solute transfer see module ‘SOLUTE TRANSPORT IN MACROPORES’ in trnsfr.f



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

<i>Surface Water Flux</i>		
$Q_{rx,y} = V_{(x,y)} d_{m(x,y)} L_{(x,y)}$	runoff downslope,	[D1a]
$Q_{rx(x+I,y)} = Q_{rx,y} S_{x(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	partition downslope runoff	
$Q_{ry(x,y+I)} = Q_{rx,y} S_{y(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	into $x$ (EW) and $y$ (NS) directions	
$Q_{s(s,w,i)(x,y)} = F u_a A_{(x,y)}$		[D1b]
$Q_{sx(s,w,i)x(x+I,y)} = Q_{(s,w,i)(x,y)} S_{x(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	snowpack snow $s$ , water $w$	
$Q_{sy(s,w,i)y(x,y+I)} = Q_{(s,w,i)(x,y)} S_{y(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	and ice $i$ transfer in downslope, $x$ (EW) and $y$ (NS) directions	
$d_{m(x,y)} = \max(0, d_{w(x,y)} + d_{i(x,y)} - d_{s(x,y)}) d_{w(x,y)} / (d_{w(x,y)} + d_{i(x,y)})$	mobile ponded water depth	[D2]
$v_{(x,y)} = R^{0.67} s_{(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity	[D3]
$\Delta(d_{w(x,y)} A_{x,y}) / \Delta t = Q_{rx(x,y)} - Q_{rx(x+I,y)} + Q_{ry(x,y)} - Q_{ry(x,y+I)} + P - E_{x,y} - Q_{wz(x,y,z=I)}$	change in ponded water depth from 2D kinematic wave theory for overland flow	[D4]
$R = d_w / 2\pi$	wetted perimeter	[D5]
$s_{x(x,y)} = 2 \text{ abs}[(Z_{x,y} + d_{sx,y} + d_{mx,y}) - (Z_{x+1,y} + d_{sx+1,y} + d_{mx+1,y})] / (L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and pooled surface water	[D6]
$s_{y(x,y)} = 2 \text{ abs}[(Z_{x,y} + d_{sx,y} + d_{mx,y}) - (Z_{x,y+1} + d_{sx,y+1} + d_{mx,y+1})] / (L_{y(x,y)} + L_{y(x,y+1)})$	in $x$ (EW) and $y$ (NS) direction	
<i>Subsurface Water Flux</i>		
$Q_{wx(x,y,z)} = K'_x (\psi_{sx,y,z} - \psi_{sx+I,y,z})$	3D Richard's or Green-Ampt equation depending on	[D7a]
$Q_{wy(x,y,z)} = K'_y (\psi_{sx,y,z} - \psi_{sx,y+I,z})$	saturation	[D7b]
$Q_{wz(x,y,z)} = K'_z (\psi_{sx,y,z} - \psi_{sx,y,z+I})$	of source or target cell in $x$ (EW), $y$ (NS) and $z$ (vertical) directions	[D7c]
$\psi_m(\theta) = -\exp[\ln(-\psi_{FC}) + \{(\ln\theta_{FC} - \ln\theta) / (\ln\theta_{FC} - \ln\theta_{WP}) * (\ln(-\psi_{FC}) - \ln(-\psi_{WP}))\}]$ ( $\theta < \theta_{FC}$ )	matric water potential from water content	[D7d]
$= -\exp[\ln(-\psi_{ST}) + \{(\ln\theta_{ST} - \ln\theta) / (\ln\theta_{ST} - \ln\theta_{FC}) * (\ln(-\psi_{ST}) - \ln(-\psi_{FC}))\}]$ ( $\theta \geq \theta_{FC}$ )		[D7e]
$\psi_s = \psi_m + \psi_\pi + \psi_g$	total soil water potential	
$\Delta\theta_{w,x,y,z} / \Delta t = (Q_{wx(x,y)} - Q_{wx+I(x,y)} + Q_{wy(x,y)} - Q_{wy+I(x,y)} + Q_{wz(x,y)} - Q_{wz+I(x,y)} + Q_{f(x,y,z)}) / L_{z(x,y,z)}$	3D water transfer plus freeze-thaw	[D8]
$K'_x = 2 K_{x,y,z} K_{x+I,y,z} / (K_{x,y,z} L_{x,(x+I,y,z)} + K_{x+I,y,z} L_{x,(x,y,z)})$	in direction $x$ if source and destination cells are unsaturated	[D9a]

$= 2 K_{x,y,z} / (L_{\alpha(x+1,y,z)} + L_{\alpha(x,y,z)})$	in direction $x$ if source cell is saturated	[D9b]
$= 2 K_{x+1,y,z} / (L_{\alpha(x+1,y,z)} + L_{\alpha(x,y,z)})$	in direction $x$ if destination cell is saturated	
$K'_y = 2 K_{x,y,z} K_{x,y+1,z} / (K_{x,y,z} L_{y(x,y+1,z)} + K_{x,y+1,z} L_{y(x,y,z)})$	in direction $y$ if source and destination cells are unsaturated	[D9a]
$= 2 K_{x,y,z} / (L_{y(x,y+1,z)} + L_{y(x,y,z)})$	in direction $y$ if source cell is saturated	[D9b]
$= 2 K_{x,y+1,z} / (L_{y(x,y+1,z)} + L_{y(x,y,z)})$	in direction $y$ if destination cell is saturated	
$K'_z = 2 K_{x,y,z} K_{x,y,z+1} / (K_{x,y,z} L_{z(x,y,z+1)} + K_{x,y,z+1} L_{z(x,y,z)})$	in direction $z$ if source and destination cells are unsaturated	[D9a]
$= 2 K_{x,y,z} / (L_{z(x,y,z+1)} + L_{z(x,y,z)})$	in direction $z$ if source cell is saturated	[D9b]
$= 2 K_{x,y,z+1} / (L_{z(x,y,z+1)} + L_{z(x,y,z)})$	in direction $z$ if destination cell is saturated	

### Exchange with Water Table

$Q_{tx(x,y,z)} = K_{x,y,z} [\psi' - \psi_{sx,y,z} + 0.0098 (d_{zx,y,z} - d_t)] / (L_{tx} + 0.5 L_{\alpha(x,y,z)})$	if $\psi_{sx,y,z} > \psi' + 0.0098(d_{zx,y,z} - d_t)$ in $x$ (EW) and $y$ (NS) directions for all depths $z$ from $d_{zx,y,z}$ to $d_t$ or if $d_{zx,y,z} > d_t$	[D10]
$Q_{ty(x,y,z)} = K_{x,y,z} [\psi' - \psi_{sx,y,z} + 0.0098 (d_{zx,y,z} - d_t)] / (L_{ty} + 0.5 L_{y(x,y,z)})$		

### Surface Heat Flux

$Rn_s + LE_s + H_s + G_s = 0$	for each ground surface $s$ including snow, litter and soil	[D11a]
$Rn_s = Rs_s + Rls_s - Rlu_s + \sum_i Rlci - \sum_i Rlgci$	ground surface net radiation	[D11b]
$LE_q = L (e_a - e_q(T_q)) / r_{aq}$	$LE$ from ground air-Atmosphere evaporation	[D11c]
$LE_s = L (e_q(T_q) - e_s(T_s, \psi_s)) / r_{as}$	$LE$ from surface-ground air evaporation	[D11d]
$H_q = \rho C_p (T_a - T_q) / r_{aq}$	$H$ from ground air-atmosphere sensible heat	[D11e]
$H_s = \rho C_p (T_q - T_s) / r_{as}$	$H$ from surface-ground air sensible heat	[D11f]

### Subsurface Heat Flux

$G_{x(x,y,z)} = 2 \kappa_{(x,y,z),(x+1,y,z)} (T_{(x,y,z)} - T_{(x+1,y,z)}) / (L_x(x,y,z) + L_x(x+1,y,z)) + c_w T_{(x,y,z)} Q_{wx(x,y,z)}$	3D conductive – convective heat flux among snowpack layers, surface litter and soil layers in $x$ (EW), $y$ (NS) and $z$ (vertical) directions	[D12a]
$G_{y(x,y,z)} = 2 \kappa_{(x,y,z),(x,y+1,z)} (T_{(x,y,z)} - T_{(x,y+1,z)}) / (L_y(x,y,z) + L_y(x,y+1,z)) + c_w T_{(x,y,z)} Q_{wy(x,y,z)}$		[D12b]
$G_{z(x,y,z)} = 2 \kappa_{(x,y,z),(x,y,z+1)} (T_{(x,y,z)} - T_{(x,y,z+1)}) / (L_z(x,y,z) + L_z(x,y,z+1)) + c_w T_{(x,y,z)} Q_{wz(x,y,z)}$		[D12c]

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

thermal conductivity of soil and surface litter [D12d]

$$\kappa_{sl}(x,y) = 0.0036 * 10^{(2.650 * \rho_{sl} - 1.652)}$$

thermal conductivity of snow layer [D12e]

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

3D general heat flux equation driving freezing-thawing in snowpack, surface litter and soil layers [D13]

## Gas Flux

$$Q_{ds\gamma x,y,z} = a_{gsx,y,z} D_{d\gamma} (S'_{\gamma} f_{d_{\gamma}x,y,z} [\gamma_{gs}]_{x,y,z} - [\gamma_{ss}]_{x,y,z})$$

volatilization – dissolution [D14a]

$$Q_{dr\gamma x,y,z} = a_{grx,y,z} D_{d\gamma} (S'_{\gamma} f_{d_{\gamma}x,y,z} [\gamma_{gr}]_{x,y,z} - [\gamma_{sr}]_{x,y,z})$$

between aqueous gaseous phases in soil and root [D14b]

$$Q_{gs\gamma z,x,y,l} = g_{ax,y} \{ [\gamma_a] - \{ 2 [\gamma_{gs}]_{x,y,l} D_{gs\gamma z(x,y,l)} / L_{z(x,y,l)} + g_{ax,y} [\gamma_a] \} / \{ 2 D_{gs\gamma z(x,y,l)} / L_{z(x,y,l)} + g_{ax,y} \} \}$$

volatilization – dissolution [D15a]

between gaseous and aqueous phases at the soil surface ( $z = l$ ) and the atmosphere [D15b]

$$Q_{ds\gamma x,y,l} = a_{gsx,y,l} D_{d\gamma} (S'_{\gamma} f_{d_{\gamma}x,y,l} [\gamma_a] - [\gamma_{ss}]_{x,y,l})$$

$$Q_{gs\gamma x(x,y,z)} = - Q_{wx(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma x(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x+l,y,z}) / (L_{x(x,y,z)} + L_{x(x+l,y,z)})$$

3D convective - conductive [D16a]

gas flux among soil layers in  $x$  (EW),  $y$  (NS) and  $z$  (vertical) directions, [D16b]

$$Q_{gs\gamma y(x,y,z)} = - Q_{wy(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma y(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y+l,z}) / (L_{y(x,y,z)} + L_{y(x,y+l,z)})$$

[D16c]

$$Q_{gs\gamma z(x,y,z)} = - Q_{wz(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma z(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y,z+l}) / (L_{z(x,y,z)} + L_{z(x,y,z+l)})$$

[D16d]

convective - conductive gas flux between roots and the atmosphere

$$Q_{gr\gamma z(x,y,z)} = D_{gr\gamma z(x,y,z)} ([\gamma_{gr}]_{x,y,z} - [\gamma_a]) / \sum_{1,z} L_{z(x,y,z)}$$

$$D_{gs\gamma x(x,y,z)} = D'_{g\gamma} f_{gx,y,z} [0.5 (\theta_{gx,y,z} + \theta_{gx+l,y,z})]^2 / \theta_{psx,y,z}^{0.67}$$

gasous diffusivity as a [D17a]

$$D_{gs\gamma y(x,y,z)} = D'_{g\gamma} f_{gy,y,z} [0.5 (\theta_{gx,y,z} + \theta_{gx,y+l,z})]^2 / \theta_{psx,y,z}^{0.67}$$

function of air-filled porosity in soil [D17b]

$$D_{gs\gamma z(x,y,z)} = D'_{g\gamma} f_{gz,y,z} [0.5 (\theta_{gx,y,z} + \theta_{gx,y,z+l})]^2 / \theta_{psx,y,z}^{0.67}$$

[D17c]

$$D_{gr\gamma z(x,y,z)} = D'_{g\gamma} f_{gx,y,z} \theta_{prx,y,z}^{1.33} A_{r(x,y,z)} / A_{x,y}$$

gasous diffusivity as a function of air-filled porosity in roots [D17d]

$$Q_{b\gamma z} = \min[0.0, \{ (44.64 \theta_{wx,y,z} 273.16 / T_{(x,y,z)}) - \Sigma_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d_{\gamma}x,y,z} M_{\gamma})) \} / ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d_{\gamma}x,y,z} M_{\gamma})) / \Sigma_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d_{\gamma}x,y,z} M_{\gamma})) S'_{\gamma} f_{d_{\gamma}x,y,z} M_{\gamma} V_{x,y,z}$$

bubbling (-ve flux) when total of all partial gas pressures exceeds atmospheric pressure [D18]

## Solute Flux

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

## Definition of Variables in Table S4

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
g	near surface ground air				
s	ground surface (snow, litter, soil)				
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	m <sup>2</sup>	[D1b,D17c]		
A <sub>r</sub>	root cross-sectional area of landscape position	m <sup>2</sup>	[D17c]		
a <sub>gr</sub>	air-water interfacial area in roots	m <sup>2</sup> m <sup>-2</sup>	[D14b]		

$a_{gs}$	air-water interfacial area in soil	$m^2 m^{-2}$	[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	$MJ m^{-2} ^\circ C^{-1}$	[D13]		
$c_w$	heat capacity of water	$MJ m^{-3} ^\circ C^{-1}$	[D12]	4.19	
$D_{d\gamma}$	volatilization - dissolution transfer coefficient for gas $\gamma$	$m^2 h^{-1}$	[D14,D15a]		
$D_{gr\gamma}$	gaseous diffusivity of gas $\gamma$ in roots	$m^2 h^{-1}$	[D16d,D17d]		Luxmoore et al. (1970a,b)
$D_{gs\gamma}$	gaseous diffusivity of gas $\gamma$ in soil	$m^2 h^{-1}$	[D15a,D16a,b,c,D17a,b,c]		Millington and Quirk (1960)
$D'_{g\gamma}$	diffusivity of gas $\gamma$ in air at 0 $^\circ C$	$m^2 h^{-1}$	[D17]	6.43 x 10 <sup>-2</sup> for $\gamma = O_2$	Campbell (1985)
$D'_{qr}$	dispersivity in roots	m	[D20d]	0.004	
$D_q$	dispersivity in soil	m	[D20,D21]		
$D_{r\gamma}$	aqueous diffusivity of gas or solute $\gamma$ in roots	$m^2 h^{-1}$	[D19d,D20d]		
$D_{s\gamma}$	aqueous diffusivity of gas or solute $\gamma$ in soil	$m^2 h^{-1}$	[D19,D20]		
$D'_{s\gamma}$	diffusivity of gas $\gamma$ in water at 0 $^\circ C$	$m^2 h^{-1}$	[D20]	8.57 x 10 <sup>-6</sup> for $\gamma = O_2$	Campbell (1985)
$d_m$	depth of mobile ponded water	m	[D1a,D2,D6]		
$d_i$	depth of surface ice	m	[D2]		
$d_s$	maximum depth of ponded water storage	m	[D2,D6]		
$d_t$	depth of external water table	m	[D10]		
$d_w$	depth of ponded water	m	[D4,D5]		
$d_z$	depth to mid-point of soil layer	m	[D10]		
$E$	evaporation or transpiration flux	$m^3 m^{-2} h^{-1}$	[D4,D11]		
$e_a$	atmospheric vapor density	$m^3 m^{-3}$	[D6,D11c]		
$e_{q(T_q)}$	ground air vapor density at current $T_q$	$g m^{-3}$	[D11c,D11d]		
$e_{s(T_s, \psi_s)}$	ground surface vapor density at current $T_s$ and $\psi_s$	$g m^{-3}$	[D11d]		
$F$	rate constant for lateral transfer of $V_{(s,w,i)}$	$h^{-1}$	[D1b]		
$f_{d\gamma}$	temperature dependence of $S'_\gamma$	-	[D14,D15b,D18]		Wilhelm et al. (1977)
$f_g$	temperature dependence of $D'_{g\gamma}$	-	[D17]		Campbell (1985)
$f_s$	temperature dependence of $D'_{s\gamma}$	-	[D20]		Campbell (1985)
$G$	soil surface heat flux	$m^3 m^{-2} h^{-1}$	[D11]		
$G_x, G_y, G_z$	soil heat flux in x, y or z directions	$MJ m^{-2} h^{-1}$	[D12,D13]		

$g_a$	boundary layer conductance	$m\ h^{-1}$	[D15a]	$(\theta < \theta_{FC})$	
$\gamma$	gas (H <sub>2</sub> O, CO <sub>2</sub> , O <sub>2</sub> , CH <sub>4</sub> , NH <sub>3</sub> , N <sub>2</sub> O, N <sub>2</sub> , H <sub>2</sub> ) or solute (from S5)		[D14,D15]		
$[\gamma_a]$	atmospheric concentration of gas $\gamma$	$g\ m^{-3}$	[D15,D16d]		
$[\gamma_{gr}]$	gaseous concentration of gas $\gamma$ in roots	$g\ m^{-3}$	[D14b,D16d]		
$[\gamma_{gs}]$	gaseous concentration of gas $\gamma$ in soil	$g\ m^{-3}$	[D14a,D15a,D16a,D16b,D16c]		
$[\gamma_{sr}]$	aqueous concentration of gas $\gamma$ in roots	$g\ m^{-3}$	[D14b, D19d]	Green and Corey (1971)	
$[\gamma_{tr}]$	aqueous concentration of gas $\gamma$ at root surface	$g\ m^{-3}$	[D19b]		
$[\gamma_{ss}]$	aqueous concentration of gas $\gamma$ in soil	$g\ m^{-3}$	[D14a,D15b,D18,D19]		
$H_q$	sensible heat flux between ground air and atmosphere	$MJ\ m^{-2}\ h^{-1}$	[D11e]		
$H_s$	sensible heat flux between ground surface and ground air	$MJ\ m^{-2}\ h^{-1}$	[D11f]		
$K$	hydraulic conductivity	$m^2\ MPa^{-1}\ h^{-1}$	[D9,D10]		
$K'_x, K'_y, K'_z$	hydraulic conductance in $x, y$ or $z$ directions	$m\ MPa^{-1}\ h^{-1}$	[D7,D9]		
$\kappa$	bulk thermal conductivity of soil layer or surface litter	$MJ\ m^{-1}\ h^{-1}\ ^\circ C^{-1}$	[D12a,b,c,d,e]		
$\kappa_{sl}$	bulk thermal conductivity of snowpack layer	$MJ\ m^{-1}\ h^{-1}\ ^\circ C^{-1}$	[D12e]		
$\kappa'_{o, m, w, i, a}$	thermal conductivity of organic matter, mineral water, ice and air	$MJ\ m^{-1}\ h^{-1}\ ^\circ C^{-1}$	[D12d]		
$L_i$	root length	$m\ m^{-2}$	[D19d]	Sturm et al. (1997)	9.05 x 10 <sup>-4</sup> , 1.06 x 10 <sup>-2</sup> , 2.07 x 10 <sup>-3</sup> , 7.84 x 10 <sup>-3</sup> , 9.05 x 10 <sup>-5</sup>
$L_t$	distance from boundary to external water table in $x$ or $y$ directions	$m$	[D10]		
$L_x, L_y, L_z$	length of landscape element in $x, y$ or $z$ directions	$M$	[D1a,D1b,D5,D8,D9,D10,D12,D15a,D16,D19]		
$LE_q$	latent heat flux from ground air to atmosphere	$MJ\ m^{-2}\ h^{-1}$	[D11c]		
$LE_s$	latent heat flux from ground surface to ground air	$MJ\ m^{-2}\ h^{-1}$	[D11d]		
$L$	latent heat of evaporation	$MJ\ m^{-3}$	[D11,D13]		
$M_\gamma$	atomic mass of gas $\gamma$	$g\ mol^{-1}$	[D18]		
$P$	precipitation flux at ground surface	$m^3\ m^{-2}\ h^{-1}$	[D4]		
$Q_{a\gamma}$	aqueous flux of gas or solute $\gamma$ in soil	$g\ m^{-2}\ h^{-1}$	[D19a,b,c]		
$Q_{b\gamma z}$	bubbling flux	$g\ m^{-2}\ h^{-1}$	[D18]		
$Q_{dr\gamma}$	volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in roots	$g\ m^{-2}\ h^{-1}$	[D14b]	2460	
$Q_{ds\gamma}$	volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in soil	$g\ m^{-2}\ h^{-1}$	[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]		
$Q_r$	surface water flow in downslope direction	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D1a]		
$Q_{\text{rx}}, Q_{\text{ry}}$	surface water flow in $x$ or $y$ directions	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D1a,D4]		
$Q_{\text{r}\gamma}$	aqueous flux of gas or solute $\gamma$ from soil and root aqueous phases to root surface	$\text{g m}^{-2} \text{h}^{-1}$	[D19d]		
$Q_{\text{s(s,w,i)}}$	downslope movement of snowpack snow $s$ , water $w$ and ice $i$	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D1b]		
$Q_{\text{sx(s,w,i)}}, Q_{\text{sy(s,w,i)}}$	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]		
$Q_{\text{wx}}, Q_{\text{wy}}, Q_{\text{wz}}$	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]		
$\theta_{\text{FC}}$	water content at field capacity	$\text{m}^3 \text{m}^{-3}$	[D7d]		
$\theta_{\text{g}}$	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	
$\theta_{\text{w}}$	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	m	[D3,D5a]		
$Rlc_{\text{ci}}$	canopy-ground surface longwave radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11b]		
$Rlg_{\text{ci}}$	ground surface-canopy longwave radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11b]		
$Rls_{\text{s}}$	sky-ground surface longwave radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11b]		
$Rlu_{\text{s}}$	ground surface-sky longwave radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11b]		
$Rn_{\text{s}}$	ground surface net radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11a,D1b]		
$Rs_{\text{s}}$	ground surface shortwave radiation	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11b]		
$r_{\text{aq}}$	atmosphere-ground air boundary layer resistance	$\text{s m}^{-1}$	[D11c,D11e]		
$r_{\text{as}}$	ground air-surface boundary layer resistance	$\text{s m}^{-1}$	[D11d,D11f]		
$r_{\text{qi},r}$	radius of root or mycorrhizal aerenchyma	m	[D19d]		

$r_{ti,r}$	root or mycorrhizal radius	m	[D19d]	$1.0 \times 10^{-4}$ or $5.0 \times 10^{-6}$	Wilhelm et al. (1977)
$r_s$	thickness of soil water films	m	[D19d, D21d]		
$\rho_{sl}$	density of snowpack layer	Mg m <sup>-3</sup>	[D12e]		
$S'_\gamma$	Ostwald solubility coefficient of gas $\gamma$ at 30 °C	-	[D14,D15b,D18]	0.0293 for $\gamma =$ O <sub>2</sub>	
$s$	slope in downhill direction	m m <sup>-1</sup>	[D3]		
$s_x, s_y$	slope in x or y directions	m m <sup>-1</sup>	[D1a,D1b,D6]		
$T$	soil temperature	K	[D12,D18]		
$T_a$	atmospheric temperature	K	[D11e]		
$T_q$	ground air temperature	K	[D11e,D11f]		
$T_s$	ground surface temperature	K	[D11d,D11f]		
$\tau$	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	m <sup>3</sup> m <sup>-2</sup>	[D1b]		
$v_x, v_y$	velocity of surface flow in x or y directions	m h <sup>-1</sup>	[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 0.611, 1.609	de Vries (1963)
$\psi_s$	soil water potential at saturation	MPa	[D10]	$5.0 \times 10^{-3}$	
$\psi_{mg}$	soil gravimetric potential	MPa	[D7e]		
$\psi_{FC}$	soil matric potential at field capacity	MPa	[D7d]	-0.03	
$\psi_m$	soil matric potential	MPa	[D7d,e]		
$\psi_{WP}$	soil matric potential at wiltng point	MPa	[D7d,e]	-1.5	
$\psi_\pi$	soil osmotic potential	MPa	[D7e]		
$\psi_s$	soil water potential	MPa	[D7,D10]		
$u_a$	wind speed	m h <sup>-1</sup>	[D1b]		
$Z$	surface elevation	m	[D1b,D5b]		
$z_s$	snowpack depth	m	[D1b]		
$z_r$	Manning's roughness coefficient	m <sup>-1/3</sup> h	[D3]	0.01	





## **S5: Soil Solute Transformations**

### *Solute Equilibria*

Solution  $[\text{NH}_4^+]$ ,  $[\text{NO}_3^-]$  and  $[\text{H}_2\text{PO}_4^-]$  that drive root, mycorrhizal [C23] and microbial [A26] nutrient uptake 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 – E16], anion exchange between adsorbed and soluble  $\text{H}_2\text{PO}_4^-$ ,  $\text{HPO}_4^{2-}$  and  $\text{OH}^-$  [E16 – E22], and carboxyl dissociation [E23]. These reactions are solved in band and non-band soil zones if banded fertilizer applications are included in the model run.

If the salt option is selected in the site file, then ion pairing [E24 – E57] and silicate weathering [E58 – E63] reactions are also modeled. In this case ( $\text{H}^+$ ) activity determined by these reactions is used to calculate soil pH. If the salt option is not selected, then [E1 – E23] are solved at the pH given in the soil file. Ion activities used in these reactions are calculated from ion concentrations multiplied by Debye-Huckel activity coefficients.

Solute concentrations from all these reactions are used to calculate soil osmotic potentials that affect microbial growth [A15], soil water transport [D7], root water uptake [B6] and hence canopy water potential [B14] and stomatal resistance [B2b]. All solutes in these reactions undergo convective-dispersive transport through, and discharge from, the soil profile [D19 – D21]. Key salt ions ( $\text{Al}^{3+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{SO}_4^{2-}$  and  $\text{Cl}^-$ ) are transferred along concentration gradients from soil through roots to leaves, in which they affect root and canopy osmotic potentials [B4], and from which they are returned to the soil through root and leaf litterfall [C18]. Ion concentrations are also used to calculate electrical conductivity for comparison with measured values.

For precipitation-dissolution, see module ‘PRECIPITATION-DISSOLUTION REACTIONS IN NON-BAND, BAND’ in solute.f

For cation exchange, see module ‘CATION EXCHANGE FROM GAPON SELECTIVITY COEFFICIENTS’ in solute.f

For anion exchange, see module ‘PHOSPHORUS ANION EXCHANGE’ in solute.f

For ion pairing, see module ‘ION PAIRING REACTIONS’ in solute.f

For silicate weathering, see module ‘SILICATE ROCK WEATHERING’ in solute.f

**Table S5: Soil Solute Transformations**

(all concentrations and activities are in mol m<sup>-3</sup>)

*Precipitation - Dissolution Equilibria*

$\text{Al}(\text{OH})_{3(s)} \leftrightarrow (\text{Al}^{3+}) + 3 (\text{OH}^-)$	(amorphous $\text{Al}(\text{OH})_3$ )	3.0E-22	[E1] <sup>1</sup>
$\text{Fe}(\text{OH})_{3(s)} \leftrightarrow (\text{Fe}^{3+}) + 3 (\text{OH}^-)$	(soil Fe)	2.8E-27	[E2]
$\text{CaCO}_{3(s)} \leftrightarrow (\text{Ca}^{2+}) + (\text{CO}_3^{2-})$	(calcite)	3.3E-03	[E3]
$\text{CaSO}_{4(s)} \leftrightarrow (\text{Ca}^{2+}) + (\text{SO}_4^{2-})$	(gypsum)	1.4E+01	[E4]
$\text{AlPO}_{4(s)} \leftrightarrow (\text{Al}^{3+}) + (\text{PO}_4^{3-})$	(variscite)	7.2E-18	[E5] <sup>2</sup>
$\text{FePO}_{4(s)} \leftrightarrow (\text{Fe}^{3+}) + (\text{PO}_4^{3-})$	(strengite)	4.8E-23	[E6]
$\text{Ca}(\text{H}_2\text{PO}_4)_{2(s)} \leftrightarrow (\text{Ca}^{2+}) + 2 (\text{H}_2\text{PO}_4^-)$	(monocalcium phosphate)	7.0E+07	[E7] <sup>3</sup>
$\text{CaHPO}_{4(s)} \leftrightarrow (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	(monetite)	1.0E-01	[E8]
$\text{Ca}_5(\text{PO}_4)_3\text{OH}_{(s)} \leftrightarrow 5 (\text{Ca}^{2+}) + 3 (\text{PO}_4^{3-}) + (\text{OH}^-)$	(hydroxyapatite)	2.0E-31	[E9]

*Cation Exchange Equilibria* <sup>4</sup>

$\text{X-Ca} + 2 (\text{NH}_4^+) \leftrightarrow 2 \text{X-NH}_4 + (\text{Ca}^{2+})$	0.10	[E10]
$3 \text{X-Ca} + 2 (\text{Al}^{3+}) \leftrightarrow 2 \text{X-Al} + 3 (\text{Ca}^{2+})$	2.00	[E11]
$\text{X-Ca} + (\text{Mg}^{2+}) \leftrightarrow \text{X-Mg} + (\text{Ca}^{2+})$	1.00	[E12]
$\text{X-Ca} + 2 (\text{Na}^+) \leftrightarrow 2 \text{X-Na} + (\text{Ca}^{2+})$	0.10	[E13]
$\text{X-Ca} + 2 (\text{K}^+) \leftrightarrow 2 \text{X-K} + (\text{Ca}^{2+})$	0.10	[E14]
$\text{X-Ca} + 2 (\text{H}^+) \leftrightarrow 2 \text{X-H} + (\text{Ca}^{2+})$	2.00	[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]

*Anion Exchange Equilibria*

$\text{X-OH}_2^+ \leftrightarrow \text{X-OH} + (\text{H}^+)$	4.5E-05	[E17]
$\text{X-OH} \leftrightarrow \text{X-O}^- + (\text{H}^+)$	1.1E-06	[E18]
$\text{X-H}_2\text{PO}_4 + \text{H}_2\text{O} \leftrightarrow \text{X-OH}_2^+ + (\text{H}_2\text{PO}_4^-)$	1.5E-01	[E19]
$\text{X-H}_2\text{PO}_4 + (\text{OH}^-) \leftrightarrow \text{X-OH} + (\text{H}_2\text{PO}_4^-)$	1.5E+07	[E20]
$\text{X-HPO}_4^- + (\text{OH}^-) \leftrightarrow \text{X-OH} + (\text{HPO}_4^{2-})$	7.5E+05	[E21]
$\text{X-OH}_2^+ + \text{X-OH} + \text{X-O}^- + \text{X-H}_2\text{PO}_4 + \text{X-HPO}_4^- + \text{X-COO}^- = \text{AEC}$		[E22]

*Organic Acid Equilibria*

$\text{X-COOH} \leftrightarrow \text{X-COO}^- + (\text{H}^+)$	1.0E-02	[E23]
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*Ion Pair Equilibria (if salt option is selected)*

$(\text{NH}_4^+) \leftrightarrow (\text{NH}_3)_{(s)} + (\text{H}^+)$	5.5E-07	[E24]]
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<sup>1</sup> Round brackets denote solute activity. Numbers denote solubility product (precipitation-dissolution, ion pairs, anion exchange), or Gapon coefficient (cation 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 between band and non-band zones..

<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.

$\text{H}_2\text{O} \leftrightarrow (\text{H}^+) + (\text{OH}^-)$	1.0E-08	[E25]
$(\text{CO}_2)_{(\text{g})} + \text{H}_2\text{O} \leftrightarrow (\text{H}^+) + (\text{HCO}_3^-)$	4.2E-04	[E26]
$(\text{HCO}_3^-) \leftrightarrow (\text{H}^+) + (\text{CO}_3^{2-})$	5.6E-08	[E27]
$(\text{AlOH}^{2+}) \leftrightarrow (\text{Al}^{3+}) + (\text{OH}^-)$	4.6E-07	[E28]
$(\text{Al}(\text{OH})_2^+) \leftrightarrow (\text{AlOH}^{2+}) + (\text{OH}^-)$	7.3E-07	[E29]
$(\text{Al}(\text{OH})_3^0) \leftrightarrow (\text{Al}(\text{OH})_2^+) + (\text{OH}^-)$	1.8E-05	[E30]
$(\text{Al}(\text{OH})_4^-) \leftrightarrow (\text{Al}(\text{OH})_3^0) + (\text{OH}^-)$	1.2E-05	[E31]
$(\text{AlSO}_4^+) \leftrightarrow (\text{Al}^{3+}) + (\text{SO}_4^{2-})$	1.6E-01	[E32]
$(\text{FeOH}^{2+}) \leftrightarrow (\text{Fe}^{3+}) + (\text{OH}^-)$	2.7E-08	[E33]
$(\text{Fe}(\text{OH})_2^+) \leftrightarrow (\text{FeOH}^{2+}) + (\text{OH}^-)$	4.5E-07	[E34]
$(\text{Fe}(\text{OH})_3^0) \leftrightarrow (\text{Fe}(\text{OH})_2^+) + (\text{OH}^-)$	2.5E-05	[E35]
$(\text{Fe}(\text{OH})_4^-) \leftrightarrow (\text{Fe}(\text{OH})_3^0) + (\text{OH}^-)$	1.2E-05	[E36]
$(\text{FeSO}_4^+) \leftrightarrow (\text{Fe}^{3+}) + (\text{SO}_4^{2-})$	7.1E-02	[E37]
$(\text{CaOH}^+) \leftrightarrow (\text{Ca}^{2+}) + (\text{OH}^-)$	1.25E+01	[E38]
$(\text{CaCO}_3^0) \leftrightarrow (\text{Ca}^{2+}) + (\text{CO}_3^{2-})$	4.2E-02	[E39]
$(\text{CaHCO}_3^+) \leftrightarrow (\text{Ca}^{2+}) + (\text{HCO}_3^-)$	1.35E+01	[E40]
$(\text{CaSO}_4^0) \leftrightarrow (\text{Ca}^{2+}) + (\text{SO}_4^{2-})$	1.2	[E41]
$(\text{MgOH}^+) \leftrightarrow (\text{Mg}^{2+}) + (\text{OH}^-)$	7.0E-01	[E42]
$(\text{MgCO}_3^0) \leftrightarrow (\text{Mg}^{2+}) + (\text{CO}_3^{2-})$	3.0E-01	[E43]
$(\text{MgHCO}_3^+) \leftrightarrow (\text{Mg}^{2+}) + (\text{HCO}_3^-)$	6.7E+01	[E44]
$(\text{MgSO}_4^0) \leftrightarrow (\text{Mg}^{2+}) + (\text{SO}_4^{2-})$	2.1	[E45]
$(\text{NaCO}_3^-) \leftrightarrow (\text{Na}^+) + (\text{CO}_3^{2-})$	4.5E-01	[E46]
$(\text{NaSO}_4^-) \leftrightarrow (\text{Na}^+) + (\text{SO}_4^{2-})$	3.3E+02	[E47]
$(\text{KSO}_4^-) \leftrightarrow (\text{K}^+) + (\text{SO}_4^{2-})$	5.0E+01	[E48]
$(\text{H}_3\text{PO}_4) \leftrightarrow (\text{H}^+) + (\text{H}_2\text{PO}_4^-)$	7.5	[E49]
$(\text{H}_2\text{PO}_4^-) \leftrightarrow (\text{H}^+) + (\text{HPO}_4^{2-})$	6.2E-05	[E50]
$(\text{HPO}_4^{2-}) \leftrightarrow (\text{H}^+) + (\text{PO}_4^{3-})$	2.1E-10	[E51]
$(\text{FeH}_2\text{PO}_4^{2+}) \leftrightarrow (\text{Fe}^{3+}) + (\text{H}_2\text{PO}_4^-)$	3.7E-03	[E52]
$(\text{FeHPO}_4^+) \leftrightarrow (\text{Fe}^{3+}) + (\text{HPO}_4^{2-})$	4.5E-02	[E53]
$(\text{CaH}_2\text{PO}_4^+) \leftrightarrow (\text{Ca}^{2+}) + (\text{H}_2\text{PO}_4^-)$	4.0E+01	[E54]
$(\text{CaHPO}_4^0) \leftrightarrow (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	1.82	[E55]
$(\text{CaPO}_4^-) \leftrightarrow (\text{Ca}^{2+}) + (\text{PO}_4^{3-})$	3.5E-04	[E56]
$(\text{MgHPO}_4^0) \leftrightarrow (\text{Mg}^{2+}) + (\text{HPO}_4^{2-})$	1.23	[E57]

*Silicate Weathering Equilibria (if salt option is selected)*

$\text{SiO}_4 - \text{Al}^{3+} + (3\text{H}^+) \rightarrow 0.75 \text{H}_4\text{SiO}_4 + (\text{Al}^{3+})$	1.0E+05	[E58]
$\text{SiO}_4 - \text{Fe}^{3+} + (3\text{H}^+) \rightarrow 0.75 \text{H}_4\text{SiO}_4 + (\text{Fe}^{3+})$	2.5E+03	[E59]
$\text{SiO}_4 - \text{Ca}^{2+} + (2\text{H}^+) \rightarrow 0.50 \text{H}_4\text{SiO}_4 + (\text{Ca}^{2+})$	1.0E+04	[E60]
$\text{SiO}_4 - \text{Mg}^{2+} + (2\text{H}^+) \rightarrow 0.50 \text{H}_4\text{SiO}_4 + (\text{Mg}^{2+})$	1.0E+04	[E61]
$\text{SiO}_4 - \text{Na}^+ + (\text{H}^+) \rightarrow 0.25 \text{H}_4\text{SiO}_4 + (\text{Na}^+)$	1.0E+02	[E62]



## **S6: Root and Canopy Symbiotic N<sub>2</sub> Fixation**

### *Diazotrophic 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 as described in S1 [A27,A28]. Respiration demand is driven by specific activity, microbial biomass  $M_n$ , and nonstructural C concentration  $[\chi_n]$  in root or branch diazotrophs [F1], and is constrained by temperature [F2] and microbial N or P status [F3]. Diazotroph 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 diazotrophs [F6b] as described in S3 [C14]. 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 in aqueous and gaseous phases (Grant, 2004) as described in S4 [D14 – D18].  $R_h$  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], with associated recycling and litterfall of microbial N and P as described in S1.

For symbiotic respiration in canopy, see module ‘CANOPY N2 FIXATION (CYANOBACTERIA)’ in grosub.f

For symbiotic respiration in roots, see module ‘ROOT N2 FIXATION (RHIZOBIA)’ in grosub.f

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

N<sub>2</sub> fixation  $V_{N_2}$  [F14] is driven by diazotroph N deficits [F12a] constrained by diazotroph growth respiration [F9] such that under large N deficits most growth respiration drives N<sub>2</sub> fixation, while under small N deficits, most growth respiration drives diazotrophic growth [F12b]. Growth respiration is calculated from total respiration [F1] constrained by accumulation of nonstructural N  $v_n$  with respect to nonstructural C and P also required for microbial growth in the root or branch diazotroph [F13]. Nonstructural N  $v_{nd}$  is the product of  $V_{N_2}$ , so that [F13] 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], so that N<sub>2</sub> fixation is constrained by the need of diazotrophs 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 diazotrophic growth [F16 – F18]. Microbial senescence drives N and P litterfall [F19 – F20].

For N<sub>2</sub> fixation in canopy, see module ‘NODULE N2 FIXATION FROM GROWTH RESPIRATION ...’ in grosub.f

For N<sub>2</sub> fixation in roots, see module ‘NODULE N2 FIXATION FROM GROWTH RESPIRATION ...’ in grosub.f

### *Diazotrophic – Root or Canopy Exchange*

Exchange of nonstructural C, N and P between roots or branches and diazotrophs is driven by concentration gradients [F21 – F23] created by generation, transfer and consumption of nonstructural C, N and P in shoots, roots, mycorrhizae and diazotrophs. Nonstructural C is generated by CO<sub>2</sub> fixation in branches ([C1 – C12]) and transferred along concentration gradients to roots [C50] and thence to diazotrophs [F21]. Nonstructural P is generated by root uptake [C23] and transferred along concentration gradients to branches [C51] and diazotrophs [F23]. Nonstructural N is generated in roots by mineral N uptake [C23] and in

diazotrophs through gaseous fixation [F14] and transferred along concentration gradients to branches [C51] and diazotrophs [F22]. Nonstructural C, N and P in diazotrophs is determined by root-diazotroph and branch-diazotroph exchange, by diazotroph respiration and fixation, and by remobilization from diazotroph litterfall [F24 – F26]. Rate constants for diazotroph-plant nonstructural C,N,P exchange [F21 – F23] are larger for rapid  $N_2$  fixers (e.g. soybean, alfalfa) and smaller for slow  $N_2$  fixers (e.g. mosses, lichens, bushes).

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 diazotroph 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 diazotrophs [F21], reducing  $\chi_n$  [F24] and hence slowing diazotroph 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 diazotroph to root or branch and of  $\chi_{rt}$  from root or branch to diazotroph, 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  $CO_2$  fixation and root P uptake. All equations in S6 are solved for diazotrophs in roots ( $i,l$ ) and branches ( $i,j$ ).

For diazotroph-canopy exchange, see module ‘TRANSFER NON-STRUCTURAL C,N,P BETWEEN BRANCH AND NODULES ...’ in grosub.f

For diazotroph-root exchange, see module ‘TRANSFER NON-STRUCTURAL C,N,P BETWEEN ROOT AND NODULES ...’ in grosub.f

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

<i>Diazotrophic Growth</i>		
$R_{\max i,l} = M_{\text{Cni},l} \mathbf{R}' [\sigma_{\text{Cni},l}] / ([\sigma_{\text{Cni},l}] + \mathbf{K}_{\sigma\mathbf{n}}) f_t f_{\text{NP}} f_{\text{CP}}$	respiration demand	[F1]
$f_t = T \{ \exp[\mathbf{B} - \mathbf{H}_a / (R T)] \} / \{ 1 + \exp[(\mathbf{H}_{\text{dl}} - ST) / (RT)] + \exp[(ST - \mathbf{H}_{\text{dh}}) / (R T)] \}$	Arrhenius function	[F2]
$f_{\text{NP}} = \min\{ [M_{\text{Nni},l}] / [\mathbf{M}_{\text{Nn}}'], [M_{\text{Pni},l}] / [\mathbf{M}_{\text{Pn}}'] \}$	N or P limitation	[F3]
$R_{i,l} = R_{\max i,l} (V_{\text{O}_2 i,l} / V_{\text{O}_2 \max i,l})$	O <sub>2</sub> limitation (roots)	[F4]
$V_{\text{O}_2 \max i,l} = 2.67 R_{\max i,l}$	O <sub>2</sub> demand (roots)	[F5]
$V_{\text{O}_2 i,l} = V_{\text{O}_2 \max i,l} [\text{O}_{2\text{ri},l}] / ([\text{O}_{2\text{ri},l}] + \mathbf{K}_{\text{O}_2\mathbf{r}})$	equilibrate O <sub>2</sub> uptake with supply (roots)	[F6a]
$= 2\pi L_{\text{ri},l} D_{\text{SO}_2} ([\text{O}_2] - [\text{O}_{2\text{ri},l}]) / \ln((r_{\text{ri},l} + r_{\text{wl}}) / r_{\text{ri},l})$		[F6b]
$R_{\text{mi},l} = \mathbf{R}_{\text{m}} M_{\text{Nni},l} f_{\text{tm}}$	maintenance respiration	[F7]
$f_{\text{tm}} = T \{ e^{[\mathbf{Bm} - \mathbf{H}_a / (R T)]} \} / \{ 1 + e^{[(\mathbf{H}_{\text{dl}} - ST) / (R T)]} \}$	Arrhenius function for $R_{\text{m}}$	[F8]
$R_{\text{gi},l} = \max\{0.0, R_{i,l} - R_{\text{mi},l}\}$	growth + fixation	[F9]
$R_{\text{si},l} = \max\{0.0, R_{\text{mi},l} - R_{i,l}\}$	respiration	[F10]
$L_{\text{Ci},l} = R_{\text{si},l} \min\{ M_{\text{Cni},l} / (2.5 M_{\text{Nni},l}), M_{\text{ni},l} / (25.0 M_{\text{Pni},l}) \}$	microbial senescence	[F11]
$L_{\text{Ci},l} = R_{\text{si},l} \min\{ M_{\text{Cni},l} / (2.5 M_{\text{Nni},l}), M_{\text{ni},l} / (25.0 M_{\text{Pni},l}) \}$	microbial C litterfall	[F11]
<i>Symbiotic N<sub>2</sub> Fixation</i>		
$R'_{\text{N}_2 i,l} = \max\{0, (M_{\text{Cni},l} [\mathbf{M}_{\text{Nn}}'] - M_{\text{Nni},l}) / \mathbf{E}_{\text{N}_2}'\}$	maximum respiration of N <sub>2</sub> fixation from diazotroph N deficit	[F12a]
$R_{\text{N}_2 i,l} = R'_{\text{N}_2 i,l} R_{\text{gi},l} / (R_{\text{gi},l} + R'_{\text{N}_2 i,l})$	actual respiration of N <sub>2</sub> fixation constrained by $R_{\text{g}}$	[F12b]
$f_{\text{CP}} = \min\{ [\sigma_{\text{Cni},l}] / (1.0 + [\sigma_{\text{Nni},l}] / \mathbf{K}_{\text{I}\sigma_{\text{Nn}}}), [\sigma_{\text{Pni},l}] / (1.0 + [\sigma_{\text{Nni},l}] / \mathbf{K}_{\text{I}\sigma_{\text{Pn}}}) \}$	C,P product inhibition of N <sub>2</sub> fixation	[F13]
$V_{\text{N}_2 i,l} = R_{\text{N}_2 i,l} \mathbf{E}_{\text{N}_2}'$	N <sub>2</sub> fixation from respiration and N <sub>2</sub> energy yield	[F14]
$U_{\sigma_{\text{Ci},l}} = (R_{\text{gi},l} - R_{\text{N}_2 i,l}) / (1 - \mathbf{Y}_{\text{n}}')$		[F15]
$\delta M_{\text{Cni},l} / \delta t = U_{i,l} \mathbf{Y}_{\text{n}}' - L_{\text{Ci},l}$	diazotroph C growth	[F16]
$\delta M_{\text{Nni},l} / \delta t = \delta M_{\text{Cni},l} / \delta t \min\{ \sigma_{\text{Nni},l} / \sigma_{\text{Cni},l}, [\mathbf{M}_{\text{Nn}}'] \} + R_{\text{N}_2 i,l}$	diazotroph N growth	[F17a]
$\delta M_{\text{Nni},l} / \delta t = M_{\text{Nni},l} / M_{\text{Cni},l} \delta M_{\text{Cni},l} / \delta t + R_{\text{N}_2 i,l}$	diazotroph N growth	[F17b]
$\delta M_{\text{Pni},l} / \delta t = \delta M_{\text{Cni},l} / \delta t \min\{ \sigma_{\text{Pni},l} / \sigma_{\text{Cni},l}, [\mathbf{M}_{\text{Pn}}'] \}$	diazotroph P growth	[F18a]
$\delta M_{\text{Pni},l} / \delta t = M_{\text{Pni},l} / M_{\text{Cni},l} \delta M_{\text{Cni},l} / \delta t$	diazotroph P growth	[F18b]
$L_{\text{Ni},l} = \text{abs}(\delta M_{\text{Nni},l} / \delta t)$	diazotroph N litterfall	[F19]



$$L_{Pi,l} = \text{abs}(\delta M_{Pni,l} / \delta t) \quad \delta M_{Pndi,l} / \delta t < 0 \quad \text{diazotroph P litterfall} \quad [\text{F20}]$$

### *Diazotroph – Root or Canopy Exchange*

$$V_{\sigma Ci,l} = \kappa (\sigma_{Cri,l} M_{Cni,l} - \sigma_{Cni,l} M_{Cri,l}) / (M_{Cni,l} + M_{Cri,l}) \quad \text{diazotroph–root or canopy C exchange} \quad [\text{F21}]$$

$$V_{\sigma Ni,l} = \kappa (\sigma_{Nri,l} \sigma_{Cni,l} - \sigma_{Nni,l} \sigma_{Cri,l}) / (\sigma_{Cni,l} + \sigma_{Cri,l}) \quad \text{diazotroph–root or canopy N exchange} \quad [\text{F22}]$$

$$V_{\sigma Pi,l} = \kappa (\sigma_{Pri,l} \sigma_{Cni,l} - \sigma_{Pni,l} \sigma_{Ci,l}) / (\sigma_{Cni,l} + \sigma_{Cri,l}) \quad \text{diazotroph–root or canopy P exchange} \quad [\text{F23}]$$

$$\delta \sigma_{Cni,l} / \delta t = V_{\sigma Ci,l} - \min\{R_{mi,l}, R_{li,l}\} - R_{N2i,l} - U_{\sigma Ci,l} + F_{LCI} L_{Ci,l} \quad \text{diazotroph nonstructural C} \quad [\text{F24}]$$

$$\delta \sigma_{Nni,l} / \delta t = V_{\sigma Ni,l} - \delta M_{Nni,l} / \delta t + V_{N2i,l} + F_{LNI} L_{Ni,l} \quad \text{diazotroph nonstructural N} \quad [\text{F25}]$$

$$\delta \sigma_{Pni,l} / \delta t = V_{\sigma Pi,l} - \delta M_{Pni,l} / \delta t + F_{LPI} L_{Pi,l} \quad \text{diazotroph nonstructural P} \quad [\text{F26}]$$

### Definition of Variables in Table S6

Variable	Definition	Units	Equations	Input Values	Reference
<b><i>B</i></b>	parameter such that $f_t = 1.0$ at $T_l = 298.15$ K		F2	25.229	
<b><i>Bm</i></b>	parameter such that $f_{\text{itm}} = 1.0$ at $T_l = 298.15$ K		F8	25.216	
<i>D<sub>sO<sub>2</sub></sub></i>	diffusivity of aqueous O <sub>2</sub>	m <sup>2</sup> h <sup>-1</sup>	F6b		
<i>E<sub>N<sub>2</sub></sub>'</i>	direct energy cost of N <sub>2</sub> fixation	g N g C <sup>-1</sup>	F12a,F14	0.25	Gutschick, (1981), Voisin et al., (2003)
<i>F<sub>LCI</sub></i>	fraction of diazotroph C litterfall remobilized as nonstructural C	-	F24		
<i>F<sub>LNI</sub></i>	fraction of diazotroph N litterfall remobilized as nonstructural N	-	F25		
<i>F<sub>LPI</sub></i>	fraction of diazotroph P litterfall remobilized as nonstructural P	-	F26		
<i>f<sub>CP</sub></i>	effect of diazotroph nonstructural C or P content on N <sub>2</sub> fixation	-	F1,F13		
<i>f<sub>NP</sub></i>	effect of diazotroph N or P content on respiration	-	F1,F3		
<i>f<sub>t</sub></i>	temperature function for diazotroph respiration	-	F1,F2		
<i>f<sub>itm</sub></i>	temperature function for diazotroph maintenance respiration	-	F7,F8		
<b><i>H<sub>a</sub></i></b>	energy of activation	J mol <sup>-1</sup>	F2,F8	62.5 x 10 <sup>3</sup>	

$H_{dh}$	energy of high temperature deactivation	J mol <sup>-1</sup>	F2	222.5 x 10 <sup>3</sup>
$H_{dl}$	energy of low temperature deactivation	J mol <sup>-1</sup>	F2	197.5 x 10 <sup>3</sup>
$K_{\sigma n}$	Michaelis-Menten constant for diazotroph respiration of $\sigma_{Cni,l}$	g g <sup>-1</sup>	F1	0.01
$K_{I\sigma C_n}$	inhibition constant for nonstructural N:C on N <sub>2</sub> fixation	g N g C <sup>-1</sup>	F13	10
$K_{I\sigma P_n}$	inhibition constant for nonstructural N:P on N <sub>2</sub> fixation	g N g P <sup>-1</sup>	F13	1000
$K_{O_2r}$	Michaelis-Menten constant for diazotroph O <sub>2</sub> uptake	g O m <sup>-3</sup>	F6a	0.064
$\kappa$	rate constant for nonstructural C,N,P exchange between root and diazotroph	h <sup>-1</sup>	F21,F22,F23	
$L_{ri,l}$	root length	m m <sup>-2</sup>	F6b	
$L_{Ci,l}$	diazotroph C litterfall	g C m <sup>-2</sup> h <sup>-1</sup>	F11,F16,F24	
$L_{Ni,l}$	diazotroph N litterfall	g N m <sup>-2</sup> h <sup>-1</sup>	F19,F25	
$L_{Pi,l}$	diazotroph P litterfall	g P m <sup>-2</sup> h <sup>-1</sup>	F20,F26	
$M_{Cni,l}$	diazotroph structural C	g C m <sup>-2</sup>	F1,F11,F12,F16 ,F17,F18,F21	
$M_{Cri,l}$	root structural C	g C m <sup>-2</sup>	F21	
$[M_{Nn}']$	maximum diazotroph structural N concentration	g N g C <sup>-1</sup>	F3,F12	0.125
$M_{Nni,l}$	diazotroph structural N	g N m <sup>-2</sup>	F7,F11,F12,F17,F19,F25	
$[M_{Nni,l}]$	diazotroph structural N concentration	g N g C <sup>-1</sup>	F3,F17a	
$[M_{Pn}']$	maximum diazotroph structural P concentration	g P g C <sup>-1</sup>	F3,F18a	0.0125
$M_{Pni,l}$	diazotroph structural P	g P m <sup>-2</sup>	F18a,F20,F26	
$[M_{Pni,l}]$	diazotroph structural P concentration	g P g C <sup>-1</sup>	F3,F11	
$[N_{2ri,l}]$	rhizosphere aqueous N <sub>2</sub> concentration	g N m <sup>-3</sup>	F12	
$[O_{2ri,l}]$	rhizosphere aqueous O <sub>2</sub> concentration	g O m <sup>-3</sup>	F6a,b	
$[O_{2l}]$	soil aqueous O <sub>2</sub> concentration	g O m <sup>-3</sup>	F6b	
$R_{gi,l}$	diazotroph growth respiration	g C m <sup>-2</sup> h <sup>-1</sup>	F9,F12,F15	
$R$	gas constant	J mol <sup>-1</sup> K <sup>-1</sup>	F2,F8	8.3143
$R'$	specific diazotroph respiration at 25°C, and non-limiting O <sub>2</sub> , $\chi_{ndi,l}$ , $v_{ndi,l}$ and $\pi_{ndi,l}$	h <sup>-1</sup>	F1	0.125

$R_{i,l}$	diazotroph respiration under ambient $O_2$	$g\ C\ m^{-2}\ h^{-1}$	F4,F9,F10,F24	
$R_m$	specific diazotroph maintenance respiration at 25°C	$g\ C\ g\ C^{-1}\ h^{-1}$	F7	
$R_{maxi,l}$	diazotroph respiration under non-limiting $O_2$	$g\ C\ m^{-2}\ h^{-1}$	F1,F4,F5	
$R_{mi,l}$	diazotroph maintenance respiration	$g\ C\ m^{-2}\ h^{-1}$	F7,F9,F10,F24	
$R'_{N_{2i,l}}$	maximum diazotroph $N_2$ respiration	$g\ N\ m^{-2}\ h^{-1}$	F12	
$R_{N_{2i,l}}$	actual diazotroph $N_2$ respiration	$g\ N\ m^{-2}\ h^{-1}$	F12,F14	
$R_{si,l}$	diazotroph 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
$\sigma_{Cni,l}$	diazotroph nonstructural C	$g\ m^{-2}$	F17a,F18a,F21,F22,F23,F24	
$[\sigma_{Cni,l}]$	diazotroph nonstructural C concentration	$g\ g^{-1}$	F1,F13	
$\sigma_{Cri,l}$	root nonstructural C	$g\ m^{-2}$	F21,F22,F23	
$\sigma_{Nni,l}$	diazotroph nonstructural N	$g\ N\ m^{-2}$	F17a,F22,F25	
$\sigma_{Nri,l}$	root nonstructural N	$g\ N\ m^{-2}$	F22	
$[\sigma_{Nni,l}]$	diazotroph concentration of nonstructural N	$g\ g^{-1}$	F13,F17a	
$\sigma_{Pni,l}$	diazotroph nonstructural P	$g\ P\ m^{-2}$	F18a,F23,F26	
$\sigma_{Pri,l}$	root nonstructural P	$g\ P\ m^{-2}$	F23	
$[\sigma_{Pni,l}]$	diazotroph concentration of nonstructural P	$g\ g^{-1}$	F13	
$T$	root or canopy temperature	K	F2,F8	
$U_{\sigma Ci,l}$	uptake of diazotroph nonstructural C for growth	$g\ C\ m^{-2}\ h^{-1}$	F15,F16,F24	
$V_{N_{2i,l}}$	$N_2$ fixation	$g\ N\ m^{-2}\ h^{-1}$	F12,F14,F25	
$V_{O_{2maxi,l}}$	$O_2$ uptake by diazotrophs under non-limiting $O_2$	$g\ O\ m^{-2}\ h^{-1}$	F4,F5,F6a	
$V_{O_{2i,l}}$	$O_2$ uptake by diazotrophs under ambient $O_2$	$g\ O\ m^{-2}\ h^{-1}$	F4,F6	
$V_{\sigma Pi,l}$	nonstructural P transfer between root and diazotroph	$g\ P\ m^{-2}\ h^{-1}$	F23,F26	
$Y_n'$	diazotroph growth yield	$g\ C\ g\ C^{-1}$	F15,F16	0.5



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

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

Hydrolysis of colonized litter, POC, humus [S1:A1a], microbial residues [S1:A1b] and adsorbed SOC [S1:A1c] is driven by biological activity (represented by heterotrophic respiration  $R_{i,f}$ ) of all active heterotrophic communities, including fermenters ( $n = f$ ). Hydrolysis products are transferred to soluble organic matter  $Q_i$  which is the substrate for respiration and uptake by microbial biomass [S1:A20-A22]. Respiration  $R_{i,f}$  of  $Q_{i,c}$  by fermenters is a Michaelis-Menten function of  $[Q_{i,c}]$  inhibited by  $O_2$  [G1]. Respiration products are partitioned among acetate ( $A_{i,c}$ ),  $CO_2$  and  $H_2$  according to Brock and Madigan (1991) [G2].  $R_{i,f}$  beyond that used for maintenance respiration drives the uptake of additional  $Q_{i,c}$  [G3] for microbial growth according to the growth yield  $Y_f$  of fermentation [G4]. This growth yield is calculated by dividing the free energy change of fermentation, adjusted for  $H_2$  product concentration [G5], by the energy required to transform  $Q_{i,c}$  into fermenter C ( $M_{i,f,j,c}$ ) [G4]. Change in  $M_{i,f,j,c}$  is thus the difference between uptake and respiration of  $Q_{i,c}$ , less losses from senescence and decomposition [G6] as for all heterotrophic microbial populations [S1:A23-A25]. This change determines active fermenter biomass  $M_{i,f,a}$  used in the following calculation of  $R_{i,f}$  [G1]. Ratios of  $M_{i,f,j,c}$  to  $M_{i,f,j,n}$  determine mineralization-immobilization of N [S1:A26]. Decomposition products  $D_{i,f,j,k}$  are partitioned to microbial residues  $Z_{i,j,k}$  and soil organic matter  $S_{i,j,k}$  [S1:A31-A39] which then undergo further hydrolysis.

For anaerobic fermenters, see module ‘RESPIRATION RATES BY HETEROTROPHIC FERMENTERS ...’ in nitro.f

### *Acetotrophic Methanogens*

The fermenter acetate product  $A_{i,c}$  [G2] is the substrate for respiration  $R_{i,m}$  by acetotrophic methanogens ( $n = m$ ) [G7]. Respiration products are partitioned between  $CH_4$  and  $CO_2$  according to Brock and Madigan (1991) [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 [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 methanogenic C ( $M_{i,m,j,c}$ ). Acetogenic methanogens in the model use acetate as their sole carbon and energy source (Smith and Mah, 1980). Change in  $M_{i,m,j,c}$  is thus the difference between uptake and respiration of  $A_{i,c}$ , less senescence and decomposition [G11]. This change determines  $M_{i,m,a}$  used in the following calculation of  $R_{i,m}$  [G7]. Mineralization, senescence and decomposition processes are the same as those for other microbial populations, as noted for fermenters above [S1].

For acetotrophic methanogens, see module ‘RESPIRATION RATES BY ACETOTROPHIC METHANOGENS ...’ in nitro.f

### *Hydrogenotrophic Methanogen*

*s*

The fermenter products  $CO_2$  and  $H_2$  (Eq. [G2]) are the substrates for respiration by hydrogenotrophic methanogens ( $n = h$ ) that drives  $CO_2$  reduction [G12]. Respiration products are partitioned between  $CH_4$  and  $H_2O$  according to Brock and Madigan (1991) [G13].  $R_h$  beyond that used for maintenance respiration drives the uptake of additional  $CO_2$  [G14] for microbial growth according to the growth yield  $Y_h$  of hydrogenotrophic methanogenesis (Brock and Madigan, 1991) [G15]. This growth yield is calculated by dividing the free energy

change of hydrogenotrophic methanogenesis, adjusted for  $H_2$  substrate concentration [G16], by the energy required to transform  $CO_2$  into hydrogenotrophic microbial C ( $M_{h,j,c}$ ). Change in  $M_{h,j,c}$  is thus the difference between uptake and respiration of  $CO_2$ , less senescence and decomposition [G17]. This change determines  $M_{h,a}$  used in the following calculation of  $R_h$  [G12]. Mineralization, senescence and decomposition processes are the same as those for other microbial populations [S1].

For hydrogenotrophic methanogens, see module ‘H2TROPIC METHANOGENS’ in nitro.f

### *Autotrophic Methanotrophs*

Methane generated by acetotrophic and hydrogenotrophic methanogens is the substrate for  $CH_4$  oxidation by autotrophic methanotrophs ( $n = t$ ) [G18]. The stoichiometry and energetics of the methanotrophic reactions [G22 – G24] are based on those of  $CH_4$  to  $CO_2$  in Brock and Madigan (1991). The oxidation of  $CH_4$  to  $CO_2$  is coupled through an energy yield with the oxidation of  $CH_4$  to organic C used in microbial respiration [G19]. The energy yield from  $CH_4$  oxidation is calculated by dividing the free energy change of  $CH_4$  oxidation by the energy required to transform  $CH_4$  into methanotrophic C ( $M_{t,j,c}$ ) [G20]. Oxygen requirements to sustain  $CH_4$  oxidation rates are then calculated from the stoichiometries of  $CH_4$  oxidation [G22 and G23] and aerobic microbial respiration [G24]. The  $O_2$  concentrations at methanotrophic microsites are then found at which active  $O_2$  uptake driven by requirements for  $CH_4$  oxidation equals spherical  $O_2$  diffusion to the microsites from the soil solution as for other aerobic microbial populations [S1:A16-A17]. The  $O_2$  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  $O_2$  transfer rates through the gaseous and aqueous phases of the soil profile [S1:D14 – D15 and D19-D21]. The ratio of  $O_2$  uptake to  $O_2$  requirement  $f_{O_2t}$  is then used to constrain  $CH_4$  oxidation rates [G21] so that  $CH_4$  oxidation is stoichiometrically coupled to  $O_2$  uptake. Growth respiration by methanotrophs is calculated as the difference between total respiration  $R_t$  [G21b and maintenance respiration  $R_{mt}$  [S1:A18-A19]. Growth respiration drives the uptake and transformation of additional  $CH_4$  into methanotrophic biomass  $M_{t,j,c}$  [G25] according to the growth yield. This yield is calculated by dividing the free energy change of  $CH_4$  oxidation (Brock and Madigan, 1991) [G18] by the energy required to construct new  $M_{t,j,c}$  from  $CH_4$  [G26]. Net growth of  $M_{t,j,c}$  is calculated as the uptake of  $CH_4 - C$  minus respiration and decomposition of assimilated C [G27]. This change determines  $M_{t,a}$  used in the following calculation of  $X'_t$  (Eq. [G18]). Mineralization, senescence 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,  $CH_4$  concentration profiles and the sensitivity of  $CH_4$  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  $CH_4$  emissions from differently amended soil columns at different temperatures (Grant, 1998b).

For autotrophic methanotrophs, see ‘METHANOTROPHS’ in nitro.f

## **Table S7: $CH_4$ Production and Consumption**

*Anaerobic Fermenters and  $H_2$  Producing Acetogens*

$R_{i,f} = \{ \mathbf{R}'_f M_{i,f,a} [Q_{i,c}] / ([Q_{i,c}] + \mathbf{K}_f (1 + [\text{O}_2] / \mathbf{K}_i)) \} f_t$	respiration by fermenters	[G1]
$Q_{i,c} \rightarrow 0.67 \text{ A}_{i,c} + 0.33 \text{ CO}_2\text{-C} + 0.11 \text{ H}_2$	partition respiration products	[G2]
$U_{i,f,c} = R_{m,i,f} + (R_{i,f} - R_{m,i,f}) (1.0 + Y_f)$	uptake of DOC by fermenters	$[R_{i,f} > R_{m,i,f}]$ [G3a]
$U_{i,f,c} = R_{i,f}$		$[R_{i,f} < R_{m,i,f}]$ [G3b]
$Y_f = -\Delta G_f / \mathbf{E}_M$	growth yield of fermentation	[G4]
$\Delta G_f = \Delta \mathbf{G}'_f + \{ \mathbf{R} \text{ T } \ln([H_2] / [\mathbf{H}_2'])^4 \}$	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	$[R_{i,f} > R_{m,i,f}]$ [G6a]
$\delta M_{i,f,j,c} / \delta t = F_j U_{i,f,c} - R_{m,i,f,j} - D_{i,f,j,c}$		$[R_{i,f} < R_{m,i,f}]$ [G6b]

### *Acetotrophic Methanogens*

$R_{i,m} = \{ \mathbf{R}'_m M_{i,m,a} [A_{i,c}] / (\mathbf{K}_m + [A_{i,c}]) \} f_t$	respiration by acetotrophic methanogens	[G7]
$A_{i,c} \rightarrow 0.50 \text{ CH}_4\text{-C} + 0.50 \text{ CO}_2\text{-C}$	partition respiration products	[G8]
$U_{i,m,c} = R_{m,i,m} + (R_{i,m} - R_{m,i,m}) (1.0 + Y_m)$	uptake by acetotrophic methanogens	$[R_{i,m} > R_{m,i,m}]$ [G9a]
$U_{i,m,c} = R_{i,m}$		$[R_{i,m} < R_{m,i,m}]$ [G9b]
$-Y_m = -\Delta \mathbf{G}'_m / \mathbf{E}_M$	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	$[R_{i,m} > R_{m,i,m}]$ [G11a]
$\delta M_{i,m,j,c} / \delta t = F_j U_{i,m,c} - R_{m,i,m,j} - D_{i,m,j,c}$		$[R_{i,m} < R_{m,i,m}]$ [G11]

### *Hydrogenotrophic Methanogens*

$R_h = \{ \mathbf{R}'_h M_{h,a} [H_2] / (\mathbf{K}_h + [H_2]) [CO_2] / (\mathbf{K}_c + [CO_2]) \} f_t$	respiration by hydrogenotrophic methanogens	[G12]
$CO_2\text{-C} + 0.67 \text{ H}_2 \rightarrow \text{CH}_4\text{-C}$	transform respiration products	[G13]
$U_{h,c} = R_{m,h} + (R_h - R_{m,h}) (1.0 + Y_h)$	uptake by hydrogenotrophic methanogens	$[R_h > R_{m,h}]$ [G14a]
$U_{h,c} = R_h$		$[R_h < R_{m,h}]$ [G14b]
$Y_h = -\Delta G_h / \mathbf{E}_C$	growth yield of hydrogenotrophic methanogenesis	[G15]
$\Delta G_h = \Delta \mathbf{G}'_h - \{ \mathbf{R} \text{ T } \ln([H_2] / [\mathbf{H}_2'])^4 \}$	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	$[R_h > R_{m,h}]$ [G17a]
$\delta M_{h,j,c} / \delta t = F_j U_{h,c} - R_{m,h,j} - D_{h,j,c}$		$[R_h < R_{m,h}]$ [G17b]

### *Autotrophic Methanotrophs*

$X'_t = \{X'_t M_{t,a} [CH_4] / (K_t + [CH_4])\} f_t$	CH <sub>4</sub> oxidation by methanotrophs under non- limiting O <sub>2</sub>		[G18]
$R'_t = X'_t Y_{tR}$	respiration by methanotrophs under non- limiting O <sub>2</sub>		[G19]
$Y_{tR} = -\Delta G'_t / E_G$	energy yield from CH <sub>4</sub> oxidation		[G20]
$X_t = X'_t f_{O_2t}$	CH <sub>4</sub> oxidation by methanotrophs under ambient O <sub>2</sub>		[G21a]
$R_t = R'_t f_{O_2t}$	respiration by methanotrophs under ambient O <sub>2</sub>		[G21b]
$CH_4-C + 4.00 O_2 \rightarrow CO_2-C + 2.0 H_2O$	O <sub>2</sub> requirements for CH <sub>4</sub> oxidation by methanotrophs		[G22]
$CH_4-C + 1.33 O_2 \rightarrow CH_2O-C + 0.167 H^+$	O <sub>2</sub> requirements for growth by methanotrophs		[G23]
$CH_2O -C + 2.67 O_2 \rightarrow CO_2-C + 1.5 H_2O$	O <sub>2</sub> requirements for respiration by methanotrophs		[G24]
$U_{t,c} = R_{mt} + (R_t - R_{mt}) (1.0 + Y_{tG})$	uptake by methanotrophs	$[R_t > R_{mt}]$	[G25a]
$U_{t,c} = R_t$		$[R_t < R_{mt}]$	[G25b]
$Y_{tG} = -\Delta G'_c / E_M$	growth yield of methanotrophy		[G26]
$\delta M_{t,j,c} / \delta t = F_j U_{t,c} - F_j R_t - D_{t,j,c}$	growth of methanotrophs	$[R_t > R_{mt}]$	[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]

### 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>M<sub>i</sub></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]		
<i>D<sub>h,j,c</sub></i>	decomposition of hydrogenotrophic methanogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G17]		
<i>D<sub>i,f,j,c</sub></i>	decomposition of fermenters and acetogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G6]		
<i>D<sub>i,m,j,c</sub></i>	decomposition of acetotrophic methanogens	g C m <sup>-2</sup> h <sup>-1</sup>	[G11]		
<i>D<sub>t,j,c</sub></i>	decomposition of autotrophic methanotrophs	g C m <sup>-2</sup> h <sup>-1</sup>	[G27]		



$E_C$	energy required to construct new $M_h$ from $CO_2$	$kJ\ g\ C^{-1}$	[G15]	25	
$E_G$	energy required to construct new $M_i$ from $CH_4$	$kJ\ g\ C^{-1}$	[G20]	25	Anthony (1982)
$E_M$	energy required to construct new $M_f$ or $M_m$ from organic C	$kJ\ g\ C^{-1}$	[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 $M_i$				
$fo_{2t}$	ratio of $O_2$ uptake to $O_2$ requirement for $CH_4$ oxidation		[G21a,b]		
$f_t$	temperature function for growth-related processes (dimensionless)		[G1,G7,G12]		
$\Delta G'_c$	free energy change of C oxidation- $O_2$ reduction	$kJ\ g\ C^{-1}$	[G26]	-37.5	Brock and Madigan (1991)
$\Delta G_f$	free energy change of fermentation	$kJ\ g\ Q_{i,c}^{-1}$	[G4,G5]		
$\Delta G'_f$	$\Delta G_f$ when $[H_2] = [H_2']$	$kJ\ g\ Q_{i,c}^{-1}$	[G5]	-4.50	Brock and Madigan (1991), Schink (1997)
$\Delta G_h$	free energy change of hydrogenotrophic methanogenesis	$kJ\ g\ CO_2-C^{-1}$	[G15,G16]		
$\Delta G'_h$	free energy change of hydrogenotrophic methanogenesis when $[H_2] = [H_2']$	$kJ\ g\ CO_2-C^{-1}$	[G16]	-11.0	Brock and Madigan (1991)
$\Delta G'_m$	free energy change of acetotrophic methanogenesis	$kJ\ g\ A_{i,c}^{-1}$	[G10]	-1.03	Brock and Madigan (1991), Schink (1997)
$\Delta G'_t$	free energy change of $CH_4$ oxidation by methanotrophs	$kJ\ g\ CH_4-C^{-1}$	[G20]	-66.5	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]	1.0	Brock and Madigan (1991)
$h$	descriptor for hydrogenotrophic methanogens in each $M_i$				
$i$	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]	0.15	
$K_f$	M-M constant for uptake of $DOC_{i,c}$ by fermenters and acetogens	$g\ C\ m^{-3}$	[G1]	12	McGill et al. (1981)
$K_i$	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	Mosey (1983), Robinson and Tiedje (1982)

$K_m$	M-M constant for uptake of $A_{i,c}$ by acetotrophic methanogens	$\text{g C m}^{-3}$	[G7]	12	Smith and Mah (1978), Zehnder et al. (1980) Conrad (1984)
$K_t$	M-M constant for uptake of $\text{CH}_4$ by methanotrophs	$\text{g C m}^{-3}$	[G18]	$1.2 \times 10^{-3}$	
$k$	descriptor for elemental fraction within each $j$ ( $j = c, n \text{ or } p$ )				
$M$	microbial communities	$\text{g C m}^{-2}$			
$M_h$	hydrogenotrophic methanogen community	$\text{g C m}^{-2}$	[G12,G17]		
$M_{i,f}$	fermenter and acetogenic community	$\text{g C m}^{-2}$	[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]	0.125	
$R_{i,f}$	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	Smith and Mah (1980)
$R_{mh,j}$	maintenance respiration by hydrogenotrophic methanogens	$\text{g C m}^{-2} \text{ h}^{-1}$	[G14,G17]		
$R_{mi,f,j}$	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 CO <sub>2</sub> uptake by $M_h$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G14,G17,G18]		
$U_{i,f,k}$	rate of DOC <sub><i>i,k</i></sub> uptake by $M_{i,f}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G3,G6]		
$U_{i,m,c}$	rate of A <sub><i>i,c</i></sub> uptake by $M_{i,m}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G9,G11]		
$U_{t,c}$	rate of CH <sub>4</sub> uptake by $M_t$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G25,G27]		
$X_t$	CH <sub>4</sub> oxidation by methanotrophs	$\text{g C m}^{-2} \text{ h}^{-1}$	[G21a,G22]		
$X'_t$	CH <sub>4</sub> oxidation by methanotrophs at saturating O <sub>2</sub>	$\text{g C m}^{-2} \text{ h}^{-1}$	[G1,G2,G4a]		
$X'_t$	specific CH <sub>4</sub> oxidation by methanotrophs at saturating O <sub>2</sub> , 30 °C and zero water potential	$\text{g C g}^{-1} \text{ h}^{-1}$	[G18]	0.375	Conrad (1984)
$Y_f$	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]		
$Y_{tG}$	biomass yield from methanotrophic growth respiration	$\text{g } M_t\text{-C g CH}_4\text{-C}^{-1}$	[G25a,G26]		
$Y_{tR}$	ratio of CH <sub>4</sub> respired vs. CH <sub>4</sub> oxidized by methanotrophs	$\text{g C g C}^{-1}$	[G19,G20]		

## S8: Soil 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  $H_2$ -producing acetogens, acetotrophic methanogens, hydrogenotrophic methanogens and methanotrophs,  $NH_4^+$  and  $NO_2^-$  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  $NH_4^+$  ([H1a]) or by immobilizing  $NH_4^+$  ([H1b]) or  $NO_3^-$  ([H1c]) as also described in S1. 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.

For mineralization/immobilization, see module 'N AND P MINERALIZATION-IMMOBILIZATION' in nitro.f

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

Heterotrophic populations derive energy for growth by oxidizing DOC ( $X_{DOCi,h}$ ) coupled with reduction of  $O_2$  and  $NO_x$ . Constraints on  $X_{DOCi,h}$  imposed by  $O_2$  uptake are solved in four steps:

- 1)  $X_{DOCi,h}$  under non-limiting  $O_2$  is calculated from active biomass and DOC concentration [H2],
- 2)  $O_2$  reduction under non-limiting  $O_2$  is calculated from 1) using a set respiratory quotient [H3],
- 3)  $O_2$  reduction under ambient  $O_2$  is calculated from radial  $O_2$  diffusion through water films of thickness determined by soil water potential [H4a] coupled with active uptake at heterotroph surfaces driven by 2) [H4b] as also described in S1.  $O_2$  diffusion and active uptake is population-specific, allowing the development of more anaerobic conditions at microbial surfaces associated with more biologically active substrates.  $O_2$  uptake by heterotrophs also accounts for competition with  $O_2$  uptake by nitrifiers, roots and mycorrhizae,
- 4)  $X_{DOCi,h}$  under ambient  $O_2$  is calculated from 2) and 3) [H5]. The energy yield of  $X_{DOCi,h}$  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  $O_2$  are not used.

For DOC oxidation, see module 'ENERGY YIELD AND  $O_2$  DEMAND FROM DOC AND ACETATE OXIDATION' in nitro.f

For  $O_2$  reduction, see module ' $O_2$  UPTAKE BY AEROBES' in nitro.f

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

Constraints imposed by  $NO_3^-$  availability on  $X_{DOCi,h}$  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  $X_{\text{DOC}_{i,h}}$  but not accepted by  $\text{O}_2$  because of diffusion limitations [H6] modelled from aqueous and gaseous convective-dispersive transport through the soil profile [S4:D14-D21],

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  $X_{\text{DOC}_{i,h}}$  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.

For nitrate reduction by denitrifiers, see module ‘NO3 REDUCTION FROM SPECIFIC REDUCTION RATE, ENERGY YIELD ...’ in `nitro.f`

For nitrite reduction by denitrifiers, see module ‘NO2 REDUCTION FROM SPECIFIC REDUCTION RATE, ENERGY YIELD ...’ in `nitro.f`

For nitrous oxide reduction by denitrifiers, see module ‘N2O REDUCTION FROM SPECIFIC REDUCTION RATE, ENERGY YIELD ...’ in `nitro.f`

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

Nitrifier populations derive energy for growth from oxidation of  $\text{NH}_3$  ( $X_{\text{NH}_3_{i,n}}$ ) coupled with reduction of  $\text{O}_2$ . Constraints on  $X_{\text{NH}_3_{i,n}}$  imposed by  $\text{O}_2$  uptake are solved in four steps:

1)  $X_{\text{NH}_3_{i,n}}$  under non-limiting  $\text{O}_2$  is calculated from active biomass and from  $\text{NH}_3$  and  $\text{CO}_2$  concentrations [H11].  $[\text{NH}_3]$  is in equilibrium with  $[\text{NH}_4^+]$  [S5:E24].

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] as also described in S1.  $\text{O}_2$  concentrations are governed by aqueous and gaseous convective-dispersive transport through the soil profile [S4:D14-D21].  $\text{O}_2$  uptake by nitrifiers also accounts for competition with  $\text{O}_2$  uptake by heterotrophic DOC oxidizers, roots and mycorrhizae,

4)  $X_{\text{NH}_3_{i,n}}$  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).

For ammonia oxidation, see module ‘NH3 OXIDATION FROM SPECIFIC OXIDATION RATE, ENERGY YIELD’ in `nitro.f`

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

Constraints on nitrifier oxidation of  $\text{NO}_2^-$  ( $X_{\text{NO}_2_{i,o}}$ ) 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.

For nitrite oxidation, see module 'NO2 OXIDATION FROM SPECIFIC OXIDATION RATE, ENERGY YIELD' in nitro.f

*Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers*

Nitrifiers can also derive energy for growth from oxidation of  $\text{NH}_3$  ( $X_{\text{NH}_3,i,n}$ ) coupled with reduction of  $\text{NO}_2^-$  ( $R_{\text{NO}_2,i,n}$ ). Constraints on nitrifier oxidation imposed by  $\text{NO}_2^-$  availability are solved in three steps:

- 1)  $R_{\text{NO}_2,i,n}$  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)  $R_{\text{NO}_2,i,n}$  under ambient  $\text{NO}_2^-$  and  $\text{CO}_2$  is calculated from step (1) [H20], competing for  $\text{NO}_2^-$  with [H18],
  - 3) additional  $X_{\text{NH}_3,i,n}$  enabled by  $R_{\text{NO}_2,i,n}$  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  $M_{i,n}$ .

For nitrite reduction by nitrifiers, see module 'AUTOTROPHIC DENITRIFICATION' in nitro.f

**Table S8: Soil Inorganic N Transformations**

*Mineralization and Immobilization of Ammonium by All Microbial Populations*

$$\begin{aligned} I_{\text{NH}_4^{i,n,j}} &= (M_{i,m,j,\text{C}} \text{C}_{\text{Nj}} - M_{i,m,j,\text{N}}) & (I_{\text{NH}_4^{i,n,j}} < 0) & \text{[H1a]} \\ I_{\text{NH}_4^{i,n,j}} &= (M_{i,m,j,\text{C}} \text{C}_{\text{Nj}} - M_{i,m,j,\text{N}}) [\text{NH}_4^+] / ([\text{NH}_4^+] + \text{K}_{\text{NH}_4^m}) & (I_{\text{NH}_4^{i,n,j}} > 0) & \text{[H1b]} \\ I_{\text{NO}_3^{i,n,j}} &= (M_{i,m,j,\text{C}} \text{C}_{\text{Nj}} - (M_{i,m,j,\text{N}} + I_{\text{NH}_4^{i,n,j}})) [\text{NO}_3^-] / ([\text{NO}_3^-] + \text{K}_{\text{NO}_3^m}) & (I_{\text{NO}_3^{i,n,j}} > 0) & \text{[H1c]} \end{aligned}$$

*Oxidation of DOC and Reduction of Oxygen by Heterotrophs*

$$\begin{aligned} X'_{\text{DOC},i,h} &= \{X'_{\text{DOC}} M_{i,h,a} [\text{DOC}_i] / ([\text{DOC}_i]) + \text{K}_{\text{Xh}}\} f_{\text{t}} & \text{[H2]} \\ R'_{\text{O}_2,i,h} &= \text{RQC } X'_{\text{DOC},i,h} & \text{[H3]} \\ R_{\text{O}_2,i,h} &= 4\pi n M_{i,h,a} D_{\text{SO}_2} ([\text{O}_{2\text{s}}] - [\text{O}_{2\text{mi},h}]) [r_{\text{m}} r_{\text{w}} / (r_{\text{w}} - r_{\text{m}})] & \text{[H4a]} \\ &= R'_{\text{O}_2,i,h} [\text{O}_{2\text{mi},h}] / ([\text{O}_{2\text{mi},h}] + \text{K}_{\text{O}_2h}) & \text{[H4b]} \\ X_{\text{DOC},i,h} &= X'_{\text{DOC},i,h} R_{\text{O}_2,i,h} / R'_{\text{O}_2,i,h} & \text{[H5]} \end{aligned}$$

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

$$\begin{aligned} R'_{\text{NO}_3,i,d} &= \text{E}_{\text{NO}_x} (R'_{\text{O}_2,i,d} - R_{\text{O}_2,i,d}) & \text{[H6]} \\ R_{\text{NO}_3,i,d} &= R'_{\text{NO}_3,i,d} [\text{NO}_3^-] / ([\text{NO}_3^-] + \text{K}_{\text{NO}_3d}) / (1.0 + ([\text{NO}_2^-] \text{K}_{\text{NO}_3d}) / ([\text{NO}_3^-] \text{K}_{\text{NO}_2d})) & \text{[H7a]} \\ R_{\text{NO}_3,i,d} &= R_{\text{NO}_3,i,d} / (1.0 + R_{\text{NO}_3,i,d} / (\text{K}_{\text{e}} V_{i,d})) & \text{[H7b]} \\ R_{\text{NO}_2,i,d} &= (R'_{\text{NO}_3,i,d} - R_{\text{NO}_3,i,d}) [\text{NO}_2^-] / ([\text{NO}_2^-] + \text{K}_{\text{NO}_2d}) / (1.0 + ([\text{N}_2\text{O}] \text{K}_{\text{NO}_2d}) / ([\text{NO}_2^-] \text{K}_{\text{N}_2\text{O}d})) & \text{[H8a]} \\ R_{\text{NO}_2,i,d} &= R_{\text{NO}_2,i,d} / (1.0 + R_{\text{NO}_2,i,d} / (\text{K}_{\text{e}} V_{i,d})) & \text{[H8b]} \\ R_{\text{N}_2\text{O},i,d} &= 2 (R'_{\text{NO}_3,i,d} - R_{\text{NO}_3,i,d} - R_{\text{NO}_2,i,d}) [\text{N}_2\text{O}] / ([\text{N}_2\text{O}] + \text{K}_{\text{N}_2\text{O}d}) & \text{[H9a]} \\ R_{\text{N}_2\text{O},i,d} &= R_{\text{N}_2\text{O},i,d} / (1.0 + R_{\text{N}_2\text{O},i,d} / (\text{K}_{\text{e}} V_{i,d})) & \text{[H9b]} \\ X_{\text{DOC},i,d} &= X_{\text{DOC},i,d} \text{ (from [H5])} + \text{F}_{\text{NO}_x} (R_{\text{NO}_3,i,d} + R_{\text{NO}_2,i,d}) + \text{F}_{\text{N}_2\text{O}} R_{\text{N}_2\text{O},i,d} & \text{[H10]} \end{aligned}$$

*Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers*

$$\begin{aligned} X'_{\text{NH}_3,i,n} &= X'_{\text{NH}_3} M_{i,n,a} \{[\text{NH}_3\text{S}] / ([\text{NH}_3\text{S}] + \text{K}_{\text{NH}_3n})\} \{[\text{CO}_2\text{S}] / ([\text{CO}_2\text{S}] + \text{K}_{\text{CO}_2})\} f_{\text{t}} & \text{[H11]} \\ R'_{\text{O}_2,i,n} &= \text{RQNH}_3 X'_{\text{NH}_3,i,n} + \text{RQC } X'_{\text{Ci},n} & \text{[H12]} \\ R_{\text{O}_2,i,n} &= 4\pi n M_{i,n,a} D_{\text{SO}_2} (r_{\text{m}} r_{\text{w}} / (r_{\text{w}} - r_{\text{m}})) ([\text{O}_{2\text{s}}] - [\text{O}_{2\text{mi},n}]) & \text{[H13a]} \\ &= R'_{\text{O}_2,i,n} [\text{O}_{2\text{mi},n}] / ([\text{O}_{2\text{mi},n}] + \text{K}_{\text{O}_2n}) & \text{[H13b]} \\ X_{\text{NH}_3,i,n} &= X'_{\text{NH}_3,i,n} R_{\text{O}_2,i,n} / R'_{\text{O}_2,i,n} & \text{[H14]} \end{aligned}$$

*Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers*

$$\begin{aligned} X'_{\text{NO}_2,i,o} &= X'_{\text{NO}_2} M_{i,o,a} \{[\text{NO}_2^-] / ([\text{NO}_2^-] + \text{K}_{\text{NO}_2o})\} \{[\text{CO}_2\text{S}] / ([\text{CO}_2\text{S}] + \text{K}_{\text{CO}_2})\} f_{\text{t}} & \text{[H15]} \\ R'_{\text{O}_2,i,o} &= \text{RQNO}_2 X'_{\text{NO}_2,i,o} + \text{RQC } X'_{\text{Ci},o} & \text{[H16]} \\ R_{\text{O}_2,i,o} &= 4\pi n M_{i,o,a} D_{\text{SO}_2} (r_{\text{m}} r_{\text{w}} / (r_{\text{w}} - r_{\text{m}})) ([\text{O}_{2\text{s}}] - [\text{O}_{2\text{mi},o}]) & \text{[H17a]} \\ &= R'_{\text{O}_2,i,o} [\text{O}_{2\text{mi},o}] / ([\text{O}_{2\text{mi},o}] + \text{K}_{\text{O}_2o}) & \text{[H17b]} \\ X_{\text{NO}_2,i,o} &= X'_{\text{NO}_2,i,o} R_{\text{O}_2,i,o} / R'_{\text{O}_2,i,o} & \text{[H18]} \end{aligned}$$

*Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers*

$$\begin{aligned} R'_{\text{NO}_2,i,n} &= \text{E}_{\text{NO}_x} (R'_{\text{O}_2,i,n} - R_{\text{O}_2,i,n}) & \text{[H19]} \\ R_{\text{NO}_2,i,n} &= R'_{\text{NO}_2,i,n} \{[\text{NO}_2^-] / ([\text{NO}_2^-] + \text{K}_{\text{NO}_2n})\} \{[\text{CO}_2\text{S}] / ([\text{CO}_2\text{S}] + \text{K}_{\text{CO}_2})\} & \text{[H20a]} \\ R_{\text{NO}_2,i,n} &= R_{\text{NO}_2,i,n} / (1.0 + R_{\text{NO}_2,i,n} / (\text{K}_{\text{e}} V_{i,n})) & \text{[H20b]} \\ X_{\text{NH}_3,i,n} &= X_{\text{NH}_3,i,n} \text{ (from [H14])} + 0.33 R_{\text{NO}_2,i,n} & \text{[H21]} \end{aligned}$$

**Definition of Variables in Table S8**

Name	Definition	Units	Equations	Input Values	Reference
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*Subscripts*

*a* 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>			
$C_{Nj}$	maximum ratio of $M_{i,m,j,N}$ to $M_{i,m,j,C}$ maintained by $M_{i,m,j}$	$\text{g N g C}^{-1}$	[H1]	0.22 and 0.13 for <i>j</i> = labile and resistant	
$[\text{CO}_{2s}]$	CO <sub>2</sub> concentration in soil solution	$\text{g C m}^{-3}$	[H11,H15,H20]		
$[\text{DOC}_i]$	concentration of dissolved decomposition products	$\text{g C m}^{-3}$	[H2]		
$D_{sO_2}$	aqueous dispersivity-diffusivity of O <sub>2</sub>	$\text{m}^2 \text{h}^{-1}$	[H4,H13,H17]		
$E_{\text{NO}_x}$	e <sup>-</sup> accepted by NO <sub>x</sub> vs. O <sub>2</sub> when oxidizing DOC	$\text{g N g O}_2^{-1}$	[H6,H19]	28/32 = 0.875	
$F_{\text{NO}_x}$	e <sup>-</sup> donated by C vs. e <sup>-</sup> accepted by NO <sub>x</sub> when oxidizing DOC	$\text{g C g N}^{-1}$	[H10]	12/28 = 0.43	
$F_{\text{N}_2\text{O}}$	e <sup>-</sup> donated by C vs. e <sup>-</sup> accepted by N <sub>2</sub> 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
$I_{\text{NH}_4^{i,n,j}}$	mineralization ( $I_{\text{NH}_4^{i,n,j}} < 0$ ) or immobilization ( $I_{\text{NH}_4^{i,n,j}} > 0$ ) of NH <sub>4</sub> <sup>+</sup> by $M_{i,n,j,C}$	$\text{g N m}^{-2} \text{h}^{-1}$	[H1]		
$I_{\text{NO}_3^{i,n,j}}$	immobilization ( $I_{\text{NO}_3^{i,n,j}} > 0$ ) of NO <sub>3</sub> <sup>-</sup> by $M_{i,n,j,C}$	$\text{g N m}^{-2} \text{h}^{-1}$	[H1]		
$K_{\text{CO}_2}$	M-M constant for reduction of CO <sub>2s</sub> 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 NH <sub>3s</sub> by nitrifiers	$\text{g NH}_4\text{-N m}^{-3}$	[H11]	0.14	Suzuki et al. (1974)
$Ke$	inhibition constant for electrons not accepted by O <sub>2</sub> and transferred to N oxides	$\text{g N m}^{-3} \text{h}^{-1}$	[H7,H8,H9,H20]	0.25	from Koike and Hattori (1975)
$K_{\text{NH}_4m}$	M-M constant for microbial NH <sub>4</sub> <sup>+</sup> uptake	$\text{g N m}^{-3}$	[H1]	0.35	
$K_{\text{NO}_2d}$	M-M constant for reduction of NO <sub>2</sub> <sup>-</sup> by denitrifiers	$\text{g N m}^{-3}$	[H7,H8]	1.4	Yoshinari et al. (1977)
$K_{\text{NO}_2n}$	M-M constant for reduction of NO <sub>2</sub> <sup>-</sup> by nitrifiers	$\text{g N m}^{-3}$	[H20]	1.4	
$K_{\text{NO}_2o}$	M-M constant for oxidation of NO <sub>2</sub> <sup>-</sup> by nitrifiers	$\text{g N m}^{-3}$	[H15]	1.4	
$K_{\text{NO}_3d}$	M-M constant for reduction of NO <sub>3</sub> <sup>-</sup> by denitrifiers	$\text{g N m}^{-3}$	[H7,H8]	1.4	Yoshinari et al. (1977);Khalil et al., 2005
$K_{\text{N}_2Od}$	M-M constant for reduction of N <sub>2</sub> O by denitrifiers	$\text{g N m}^{-3}$	[H9]	0.14	Yoshinari et al. (1977);Khalil et al., 2005
$K_{\text{O}_2h}$	M-M constant for reduction of O <sub>2s</sub> by heterotrophs	$\text{g O}_2 \text{m}^{-3}$	[H4b]	0.064	Griffin (1972)
$K_{\text{O}_2n}$	M-M constant for reduction of O <sub>2s</sub> by NH <sub>3</sub> oxidizers	$\text{g O}_2 \text{m}^{-3}$	[H13b]	= $K_{\text{O}_2h}$	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]	$= K_{O_2h}$	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	$g\ C\ m^{-2}$	[H1]		
	$M_{i,m,j}$				
$M_{i,m,j,N}$	N biomass of microbial population	$g\ N\ m^{-2}$	[H1]		
	$M_{i,m,j}$				
$M_{i,o,a}$	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]		
<b>RQC</b>	respiratory quotient for reduction of $O_2$ coupled to oxidation of C	$g\ O_2\ g\ C^{-1}$	[H3,H12,H16]	2.67	Brock and Madigan (1991)
<b>RQ<math>_{NH_3}</math></b>	respiratory quotient for reduction of $O_2$ coupled to oxidation of $NH_{3S}$	$g\ O_2\ g\ N^{-1}$	[H12]	3.43	Brock and Madigan (1991)
<b>RQ<math>_{NO_2}</math></b>	respiratory quotient for reduction of $O_2$ coupled to oxidation of $NO_2^-$	$g\ O_2\ g\ N^{-1}$	[H16]	1.14	Brock and Madigan (1991)
$r_m$	radius of microbial sphere	m	[H4,H13,H17]		
$r_w$	radius of $r_m$ + water film at current soil water potential	m	[H4,H13,H17]		from $\psi_s$ according to Kemper (1966)
$V_i$	soil water volume occupied by substrate-microbe complex		[7,H8,H9,H20]		
$X'_{Ci,n}$	rate of C oxidation by $NH_3$ oxidizers under non-limiting $[O_{2S}]$	$g\ C\ m^{-2}\ h^{-1}$	[H12]		
$X'_{Ci,o}$	rate of C oxidation by $NO_2^-$ oxidizers under non-limiting $[O_{2S}]$	$g\ C\ m^{-2}\ h^{-1}$	[H16]		
<b>X'DOC</b>	specific rate of DOC oxidation by heterotrophs at 25 °C under non-limiting [DOC] and $[O_{2S}]$	$g\ C\ g\ C^{-1}\ h^{-1}$	[H2]	0.125	Shields et al. (1973)
$X'_{DOCi,h}$	rate of DOC oxidation by heterotrophs under non-limiting $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H2,H3,H5]		
$X_{DOCi,h}$	rate of DOC oxidation by heterotrophs under ambient $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H5]		
$X_{DOCi,d}$	rate of DOC oxidation by heterotrophs under ambient $[O_{2S}]$ and $[NO_x]$	$g\ N\ m^{-2}\ h^{-1}$	[H10]		
<b>X'NH<math>_3</math></b>	specific rate of $NH_3$ oxidation by $NH_3$ oxidizers at 25 °C under non-limiting $[O_{2S}]$	$g\ N\ g\ C^{-1}\ h^{-1}$	[H11]]	0.375	Belser and Schmidt (1980)
$X_{NH_3i,n}$	rate of $NH_3$ oxidation by $NH_3$ oxidizers coupled with reduction of $O_2 + NO_2^-$ under ambient $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H14,H21]		
$X'_{NH_3i,n}$	rate of $NH_3$ oxidation by $NH_3$ oxidizers under non-limiting $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H11,H12,H14]		
$X'_{NO_2i,o}$	rate of $NO_2^-$ oxidation by $NO_2^-$ oxidizers under non-limiting $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H15,H16,H18]		
$X_{NO_2i,o}$	rate of $NO_2^-$ oxidation by $NO_2^-$ oxidizers coupled with reduction of $O_2$ under ambient $[O_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H18]		
<b>X'no<math>_2</math></b>	specific rate of $NO_2^-$ oxidation by $NO_2^-$ oxidizers at 25 °C under non-limiting $[O_{2S}]$	$g\ N\ g\ C^{-1}\ h^{-1}$	[H15]	0.25	Belser (1977)

## **S9: Soil Erosion**

The soil erosion model in *ecosys* is derived from the European Soil Erosion model (EUROSEM) that simulates sediment transport, erosion and deposition over the land surface during single storm events (Morgan et al., 1998). The key erosion processes in this model are sediment detachment by rainfall and overland flow, and sediment deposition and transport. These processes are coupled with those for water infiltration, ponding and runoff described in S4. Sustained soil erosion causes loss of all soil constituents, resulting in surface subsidence and reduced soil water and nutrient retention (Fig. 3), and so can cause loss in plant productivity over time.

### *Sediment Detachment by Rainfall*

Detachment by rainfall is calculated from soil detachability, rainfall kinetic energy at the ground surface, and the depth of ponded surface water (from [D2] in S4) [I1], accounting for rock, snow and ice surfaces. Detachability is determined by soil texture and organic matter content [I2] and kinetic energy by intensity of precipitation from direct throughfall and leaf drainage [I3 – I5].

For rainfall detachment, see module ‘DETACHMENT BY RAINFALL’ in erosion.f

### *Sediment Detachment/Deposition by Overland Flow*

Detachment/deposition by overland flow is calculated from the difference between the sediment transport capacity and the sediment concentration in the overland flow [I6]. Detachment is multiplied by a flow detachment efficiency coefficient [I7] that declines with soil cohesion which increases with soil surface clay, SOC, root length density and ice content. Deposition is multiplied by a sediment sinking velocity that decreases with water viscosity, and increases with average particle density and size in the soil surface layer. Sediment transport capacity [I8] is calculated from stream power in turn calculated from slope and runoff velocity from [S4:D3], and varies with average particle size in the soil surface layer [I10-I11].

For overland flow detachment, see module ‘DETACHMENT IN SURFACE WATER’ in erosion.f

For overland flow deposition, see module ‘DEPOSITION OF SEDIMENT TO SOIL SURFACE’ in erosion.f

### *Sediment Transport*

Sediment transport downslope [I12] is calculated from sediment concentration multiplied by surface runoff from [S4:D1a]. Transport downslope is partitioned into east-west *x* and north-south *y* directions according to their relative slopes [I12]. Sediment concentration is calculated from sediment amount divided by surface water volume [I13], determined by ponded water depth from [S4:D4]. Sediment amount is driven by sediment detachment, deposition and transport [I14].

For sediment transport, see module 'TRANSPORT OF SEDIMENT IN OVERLAND FLOW' in erosion.f

**Table S9: Soil Erosion**

*Sediment Detachment by Rainfall*

$D_R = k KE e^{-zd}$	sediment detachment by rainfall	[I1]
$k = 1.0^{-06} (1.0 + 2.0 (1.0 - C_{silt} - C_{soc}))$	soil detachability	[I2]
$KE = KE_{dt} + KE_{ld}$	rainfall kinetic energy at ground surface	[I3]
$KE_{dt} = (8.95 + (8.44 \log R_i)) R_t$	rainfall kinetic energy from direct throughfall	[I4]
$KE_{ld} = (15.8H^{0.5} - 5.87) R_l$	rainfall kinetic energy from leaf drainage	[I5]

*Sediment Detachment/Deposition by Overland Flow*

$D_F = \beta w (C_{Tsed} - C_{sed})$	$C_{Tsed} > C_{sed}$	sediment detachment by overland flow	[I6a]
$D_F = v_s w (C_{Tsed} - C_{sed})$	$C_{Tsed} < C_{sed}$	sediment deposition by overland flow	[I6b]
$\beta = 0.79 e^{-0.85J}$		flow detachment efficiency coefficient	[I7]
$C_{Tsed} = \rho_s c \max\{0, \omega - \omega_{cr}\}^\eta$		sediment transport capacity	[I8]
$\omega = 100 v s$		stream power	[I9]
$c = [(d50 + 5) / 0.32]^{-0.6}$		parameter in $C_{Tsed}$	[I10]
$\eta = [(d50 + 5) / 300]^{0.25}$		parameter in $C_{Tsed}$	[I11]

*Sediment Transport*

$T_{sed(x,y)} = C_{sed(x,y)} Q_{r(x,y)}$	downslope sediment transport	[I12]
$T_{sedx(x+I,y)} = T_{sed(x,y)} S_{x(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	partition downslope transport into $x$ (EW)	
$T_{sedy(x,y+I)} = T_{sed(x,y)} S_{y(x,y)} / (S_{x(x,y)} + S_{y(x,y)})$	and $y$ (NS) directions	
$C_{sed(x,y)} = sed_{(x,y)} / (d_{w(x,y)} A_{x,y})$	sediment concentration in surface water	[I13]
$sed_{(x,y)t} = sed_{(x,y)t-I} + D_F(x,y) + D_R(x,y) + T_{sedx(x,y)}$ $- T_{sedx(x+I,y)} + T_{sedy(x,y)} - T_{sedy(x,y+I)}$	change in sediment amount	[I14]

**Definition of Variables in Table S9**

Name	Definition	Units	Equations	Input	Referen
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*Subscripts*

*Variables*

$A$	area of landscape position	$m^2$			[I13]
$\beta$	flow detachment efficiency coefficient	-			[I6,I7]

$C_{\text{silt}}$	soil surface silt concentration	$\text{Mg Mg}^{-1}$	[I2]
$C_{\text{soc}}$	soil surface SOC concentration	$\text{Mg Mg}^{-1}$	[I2]
$C_{\text{sed}}$	sediment concentration	$\text{Mg m}^{-3}$	[I6,I13]
$C_{T\text{sed}}$	sediment transport capacity	$\text{Mg m}^{-3}$	[I6,I8]
$D_F$	sediment detachment/deposition by overland flow	$\text{Mg m}^{-2} \text{ h}^{-1}$	[I6,I14]
$D_R$	sediment detachment by rainfall	$\text{Mg m}^{-2} \text{ h}^{-1}$	[I1,I14]
$d$	surface water layer depth from S4 [D2]	m	[I1]
$d_{50}$	average particle size	$\mu$	[I10,I11]
$d_w$	depth of ponded water from S4 [D4]	m	[I13]
$J$	soil cohesion	kPa	[I7]
$KE$	rainfall kinetic energy at ground surface	$\text{J m}^{-2}$	[I1,I3]
$KE_{\text{dt}}$	rainfall kinetic energy from direct throughfall	$\text{J m}^{-2}$	[I3,I4]
$KE_{\text{ld}}$	rainfall kinetic energy from leaf drainage	$\text{J m}^{-2}$	[I3,I5]
$k$	soil detachability	$\text{Mg J}^{-1}$	[I1,I2]
$\rho_s$	soil particle density	$\text{Mg m}^{-3}$	[I8]
$Q_r$	surface water flow in downslope direction from S4 [D1]	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[i12]
$R_i$	incoming precipitation	$\text{mm h}^{-1}$	[I4]
$R_t$	throughfall precipitation	$\text{mm h}^{-1}$	[I4]
$R_l$	leaf drainage	$\text{mm h}^{-1}$	[I5]
$s$	slope in downhill direction	$\text{m m}^{-1}$	[I9]
$s_x, s_y$	slope in x or y directions	$\text{m m}^{-1}$	[I12]
$\text{sed}$	sediment amount	$\text{Mg m}^{-2}$	[I13,I14]
$T_{\text{sed}}$	downslope sediment transport	$\text{Mg m}^{-2} \text{ h}^{-1}$	[I12,I14]
$v$	runoff velocity from S4 [D3]	$\text{m s}^{-1}$	[I9]
$v_s$	sediment sinking velocity	$\text{m h}^{-1}$	[I6]
$w$	flow width	m	[I6]
$\omega$	stream power	$\text{cm s}^{-1}$	[I8,I9]
$\omega_{\text{cr}}$	critical stream power	$\text{cm s}^{-1}$	[I8]
0.4	Morgan et al., 1998		
$z$	exponent	-	[I1]
2.0	Morgan et al., 1998		

## **S10: Canopy and Soil Fire**

### *Ignition*

Fires are ignited by a prescribed input of longwave radiation that, when added to sky longwave radiation, raises net radiation at canopy [B1b], snowpack, litter and soil surfaces [D11b] (Fig. 1a). This rise causes more rapid energy exchange [S2:B1a,S4:D11a], driving latent [S2:B1c,d,S4:D11b,c] and sensible [S2:B1f,g,S4:D11e,f] heat loss, and surface heating [S4:D11a]. Surface heating also drives greater heat flux into the soil profile [S4:D12 – D13], raising soil temperatures. If warming causes surface or soil temperatures to exceed ignition thresholds, combustion of organic material is initiated and continues until either surface or soil temperatures decline below ignition thresholds, or the organic material is fully combusted. The rate of combustion depends upon specific combustion rates for each combustible material, including organic matter (nonstructural, non-woody, woody, roots, standing dead) [J1a] and charcoal [J1b] in each canopy, and litter, humus [J1a] and charcoal [J1b] in each soil

layer. Combustion rate increases with surface temperature above the ignition threshold [J2a,b], based on Huang and Rein (2016).

For fire ignition see module 'FIRE IGNITION' in watsub.f

For combustion in canopies and roots see module 'IF FIRE EVENT IS IN PROGRESS' in grosb.f

For combustion in soils see module 'IF FIRE EVENT IS IN PROGRESS' in nitro.f

### *Combustion Products*

Allocation of C, N and P from combusted material to mineral products (charcoal,  $\text{NH}_4^+$ ,  $\text{H}_2\text{PO}_4^-$ ) declines with increasing combustion temperature while that to gaseous products ( $\text{CO}_2$ ,  $\text{CH}_4$ ,  $\text{NO}_x$ ,  $\text{PO}_x$ ) increases [J3 – J6], as found experimentally (Gray and Dighton, 2006; Qian et al., 2009). The total combustion rate of organic material in all plant canopies, or in each soil layer [J7] drives  $\text{O}_2$  demand [J8], which drives  $\text{O}_2$  consumption depending on canopy or soil  $\text{O}_2$  concentration [J9].  $\text{O}_2$  consumption drives aerobic C combustion [J10] to generate  $\text{CO}_2$ , while the  $\text{O}_2$  demand not met by  $\text{O}_2$  consumption drives anaerobic combustion to generate  $\text{CH}_4$  [J11]. This  $\text{CH}_4$  may be combusted depending on gaseous  $\text{CH}_4$  and  $\text{O}_2$  concentrations in canopy or soil air [J12], causing further  $\text{O}_2$  consumption [J13]. Combusted C material not released as  $\text{CO}_2$  or  $\text{CH}_4$  is allocated to charcoal [J14].

Canopy air  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{CH}_4$  concentrations in [J9] and [J12] are calculated from net exchange of  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{CH}_4$  through lower boundaries with snowpack, litter and soil surfaces, through within-canopy boundaries with living and dead plant surfaces [C1 – C17], and through upper boundaries with the atmosphere. Soil air  $\text{CO}_2$ ,  $\text{O}_2$  and  $\text{CH}_4$  concentrations in [J9] and [J12] are calculated from vertical and lateral transfers in gaseous and aqueous phases between adjacent layers [S4:D14 – D20], and from net exchanges between aqueous phases and microbial biomasses within each soil layer [S1:A11 – A25].

For combustion products in canopies and roots, see module 'FIRE' in extract.f

For combustion products in soil, see module 'FIRE' in redist.f

### *Combustion Heat*

Total heat released by combustion in each living and dead canopy and in each soil layer is the sum of heat from combustion of organic and charcoal material generating  $\text{CO}_2$  and  $\text{CH}_4$ , and from combustion of  $\text{CH}_4$  generating  $\text{O}_2$  and  $\text{CO}_2$  using specific energy yields for each combustion [J15]. This heat is added to canopy or soil layer air to raise temperatures and hence latent [S2:B1c,d,S4:D11b,c] and sensible [S2:B1f,g,s4:D11e,f] heat exchange and conductive-convective heat transfer [S4:D12] when solving canopy [S1:B1a], litter or soil energy balances [s4:D11a]. These transfers raise canopy, litter and soil temperatures, thereby sustaining combustion.

For addition of canopy combustion heat to canopy air see top of module 'CONVERGENCE SOLUTION FOR CANOPY ENERGY BALANCE AND WATER UPTAKE' in uptake.f

For addition of soil combustion heat to soil see module ‘FIRE IGNITION’ in watsub.f

**Table S10: Canopy and Soil Fire**

*Ignition*

$$C_o = C'_o f_{to} \quad \text{combustion of C from organic material } o \text{ in soil or plant} \quad [J1a]$$

$$C_c = C'_c f_{tc} \quad \text{combustion of C from charcoal material } c \text{ in soil or plant} \quad [J1b]$$

$$f_{to} = \exp[B - H_o / (RT_o)] \quad T_o > T_c \quad \text{temperature dependence of organic C combustion} \quad [J2a]$$

$$f_{tc} = \exp[B - H_c / (RT_c)] \quad T_c > T_c \quad \text{temperature dependence of charcoal C combustion} \quad [J2b]$$

*Allocation of Combustion Products*

$$F_{Com} = F_{Comx} (1.0 - \min(1.0, f_{to})) \quad \text{fraction of } C_o \text{ combusted with O}_2 \text{ allocated to charcoal} \quad [J3a]$$

$$F_{Cog} = 1.0 - F_{Com} \quad \text{fraction of } C_o \text{ combusted with O}_2 \text{ allocated to CO}_2 \quad [J3b]$$

$$F_{Ccm} = F_{Ccmx} (1.0 - \min(1.0, f_{tc})) \quad \text{fraction of } C_o \text{ combusted without O}_2 \text{ allocated to charcoal} \quad [J4a]$$

$$F_{Ccg} = 1.0 - F_{Ccm} \quad \text{fraction of } C_o \text{ combusted without O}_2 \text{ allocated to CH}_4 \quad [J4b]$$

$$F_{Cnm} = F_{Cnmy} + (F_{Cnmx} - F_{Cnmy}) (1.0 - \min(1.0, f_{to})) \quad \text{fraction of combusted N allocated to NH}_4^+ \quad [J5a]$$

$$F_{Cng} = 1.0 - F_{Cnm} \quad \text{fraction of combusted N allocated to gaseous NO}_x \quad [J5b]$$

$$F_{Cpm} = F_{Cpmy} + (F_{Cpmx} - F_{Cpmy}) (1.0 - \min(1.0, f_{to})) \quad \text{fraction of combusted P allocated to H}_2\text{PO}_4^- \quad [J6a]$$

$$F_{Cpg} = 1.0 - F_{Cpm} \quad \text{fraction of combusted P allocated to gaseous PO}_x \quad [J6b]$$

$$C'_c = \Sigma_o C_o + \Sigma_c C_c \quad \text{total combustion of C from all organic + charcoal material} \quad [J7]$$

$$C'_o = 32/12 C'_c \quad \text{total O}_2 \text{ demand from } C'_c \quad [J8]$$

$$C_o = C'_o [O_2] / ([O_2] + K_{O2}) \quad \text{O}_2 \text{ limited O}_2 \text{ consumption from } C'_c \quad [J9]$$

$$C_c = 12/32 C_o \quad \text{total C combustion using O}_2 \text{ to generate CO}_2 \quad [J10]$$

$$C_H = (C'_c F_{Cog} - C_c) F_{Ccg} \quad \text{total C combustion not using O}_2 \text{ to generate CH}_4 \quad [J11]$$

$$C_{CH4} = C_H [CH_4] / ([CH_4] + K_{CH4}) [O_2] / ([O_2] + K_{O2}) \quad \text{CH}_4 \text{ and O}_2 \text{ limited CH}_4 \text{ combustion of } C_H \quad [J12]$$

$$C_{OCH4} = 32/12 C_{CH4} \quad \text{O}_2 \text{ consumption from CH}_4 \text{ combustion} \quad [J13]$$

$$F_{Cc} = (C'_c - C_c - C_H) / C'_c \quad \text{fraction of } C'_c \text{ allocated to charcoal} \quad [J14]$$

*Energy Yield from Combustion*



$$G_C = G_C C_C + G_H C_H + G_{CH_4} C_{CH_4} \text{ total energy yield from } C_C, C_H \text{ and } C_{CH_4} \text{ [J15]}$$

### Definition of Variables in Table S10

Name	Definition	Units	Equations	Input	Notes
<i>Subscripts</i>					
<i>c</i>	charcoal in canopies and soils				
<i>o</i>	organic biomass in canopies (nonstructural, non-woody, woody, roots, standing dead) and soils (litter and humus)				
<i>Variables</i>					
<b><i>B</i></b>	exponent in $f_{to}, f_{ic}$		[J2a,b]	12.03	
$C_o$	C combustion rate of charcoal material <i>c</i>	g C m <sup>-2</sup> h <sup>-1</sup>	[J1b]		
$C_o$	C combustion rate of organic material <i>o</i>	g C m <sup>-2</sup> h <sup>-1</sup>	[J1a]		
$C_C$	total C combustion using O <sub>2</sub> to generate CO <sub>2</sub>	g C m <sup>-2</sup> h <sup>-1</sup>	[J10,J11,J14,J15]		
$C'_C$	total combustion of C from all organic + charcoal material	g C m <sup>-2</sup> h <sup>-1</sup>	[J7,J8,J11,J14]		
$C'_c$	C combustion rate of charcoal material <i>c</i> when $f_{ic} = 1$	g C m <sup>-2</sup> h <sup>-1</sup>	[J1b]		500 – 1000
$C_{CH_4}$	CH <sub>4</sub> and O <sub>2</sub> limited CH <sub>4</sub> combustion of C <sub>H</sub>	g C m <sup>-2</sup> h <sup>-1</sup>	[J12,J13,J15]		
$C_H$	total C combustion not using O <sub>2</sub> to generate CH <sub>4</sub>	g C m <sup>-2</sup> h <sup>-1</sup>	[J11,J12,J14,J15]		
$C_O$	O <sub>2</sub> limited O <sub>2</sub> consumption from $C'_C$	g O m <sup>-2</sup> h <sup>-1</sup>	[J9,J10]		
$C_{OCH_4}$	O <sub>2</sub> consumption from CH <sub>4</sub> combustion	g O m <sup>-2</sup> h <sup>-1</sup>	[J13]		
$C'_O$	total O <sub>2</sub> demand from $C'_C$	g O m <sup>-2</sup> h <sup>-1</sup>	[J8,J9]		
$C'_o$	C combustion rate of organic material <i>o</i> when $f_{to} = 1$	g C m <sup>-2</sup> h <sup>-1</sup>	[J1a]		500 – 1000
[CH <sub>4</sub> ]	CH <sub>4</sub> concentration in canopy or soil air	umol mol <sup>-1</sup>	[J12]		
$F_{Cc}$	fraction of $C'_C$ allocated to charcoal		[J14]		
$F_{Ccg}$	fraction of $C_c$ combusted without O <sub>2</sub> allocated to charcoal		[J4b,J11]		
$F_{Ccm}$	fraction of $C_c$ combusted without O <sub>2</sub> allocated to charcoal		[J4a,J4b]		
$F_{Ccmx}$	maximum fraction of $C_c$ combusted without O <sub>2</sub> allocated to charcoal when $f_{to} = 0$		[J4a]		0.5
$F_{Cng}$	fraction of combusted $N_o$ allocated to gaseous NO <sub>x</sub>		[J5b]		
$F_{Cnm}$	fraction of combusted $N_o$ allocated to NH <sub>4</sub> <sup>+</sup>		[J5a,J5b]		

$F_{Cnmx}$	maximum fraction of combusted $N_o$ allocated to $NH_4^+$ when $f_{to} = 0$		[J5a]	0.4
$F_{Cnmy}$	minimum fraction of combusted $N_o$ allocated to $NH_4^+$ when $f_{to} \geq 1$		[J5a]	0.1
$F_{Cog}$	fraction of $C_o$ combusted with $O_2$ allocated to $CO_2$		[J3b,J11]	
$F_{Com}$	fraction of $C_o$ combusted with $O_2$ allocated to charcoal		[J3a,J3b]	
$F_{Comx}$	maximum fraction of $C_o$ combusted with $O_2$ allocated to charcoal when $f_{to} = 0$		[J3a]	0.0
$F_{Cpg}$	fraction of combusted $P_o$ allocated to gaseous POx		[J6b]	
$F_{Cpm}$	fraction of combusted $N_o$ allocated to $H_2PO_4^-$		[J6a,J6b]	
$F_{Cpmx}$	maximum fraction of combusted $P_o$ allocated to $H_2PO_4^-$ when $f_{to} = 0$		[J6a]	0.9
$F_{Cpmy}$	minimum fraction of combusted $P_o$ allocated to $H_2PO_4^-$ when $f_{to} \geq 1$		[J6a]	0.7
$f_{tc}$	temperature sensitivity of $C'_c$		[J1b,J2b,J4a]	
$f_{to}$	temperature sensitivity of $C'_o$		[J1a,J2a,J3a,J5a,J6a]	
$G_C$	total energy yield from $C_C$ , $C_H$ and $C_{CH4}$	$MJ\ h^{-1}$	[J15]	
$G_C$	specific energy yield from $C_C$	$MJ\ g^{-1}$	[J15]	0.0375
$G_{CH4}$	specific energy yield from $C_{CH4}$	$MJ\ g^{-1}$	[J15]	0.0743
$G_H$	specific energy yield from $C_H$	$MJ\ g^{-1}$	[J15]	0.0125
$H_c$	activation energy of $f_{tc}$ $f_{tc} = 1$ at 700 K	$J\ mol^{-1}$	[J2b]	$120 \times 10^3$
$H_o$	activation energy of $f_{to}$ $f_{to} = 1$ at 600 K	$J\ mol^{-1}$	[J2a]	$60 \times 10^3$
$K_{CH4}$	half-saturation constant for $CH_4$ combustion in canopy or soil air	$umol\ mol^{-1}$	[J12]	10
$K_{O2}$	half-saturation constant for $O_2$ consumption in canopy or soil air	$umol\ mol^{-1}$	[J9,J12]	21000 Fang et al. (2006)
$[O_2]$	oxygen concentration in canopy or soil air	$umol\ mol^{-1}$	[J9,J12]	
$R$	gas constant	$J\ mol^{-1}\ K^{-1}$	[J2a,b]	8.3143
$T_c$	threshold temperature for combustion	K	[J2a,b]	473.15 K
$T_c$	temperature of charcoal material $c$	K	[J2b]	
$T_o$	temperature of organic material $o$	K	[J2a]	

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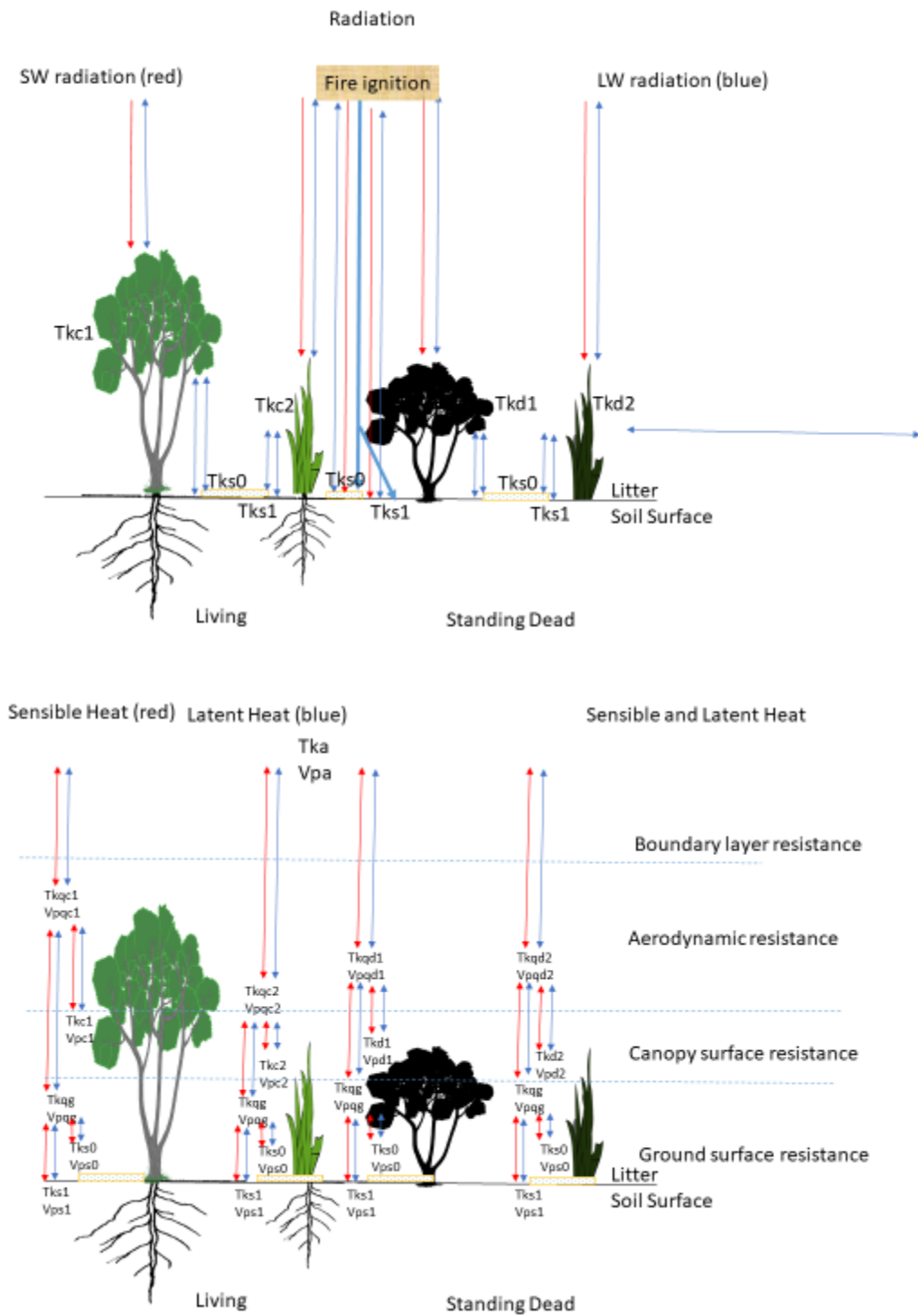


Fig. 1: (a) Radiation and (b) aerodynamic and surface heat fluxes modelled in *ecosys*

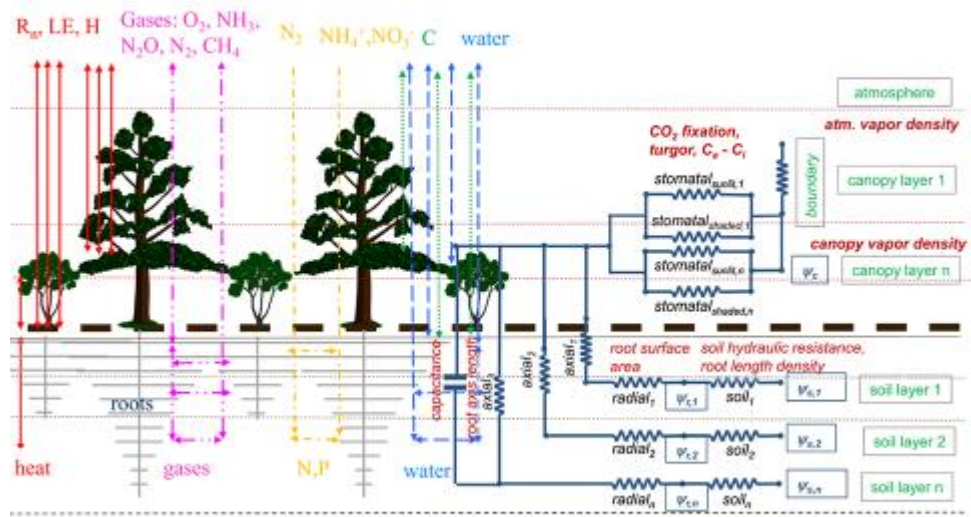


Fig. 2.



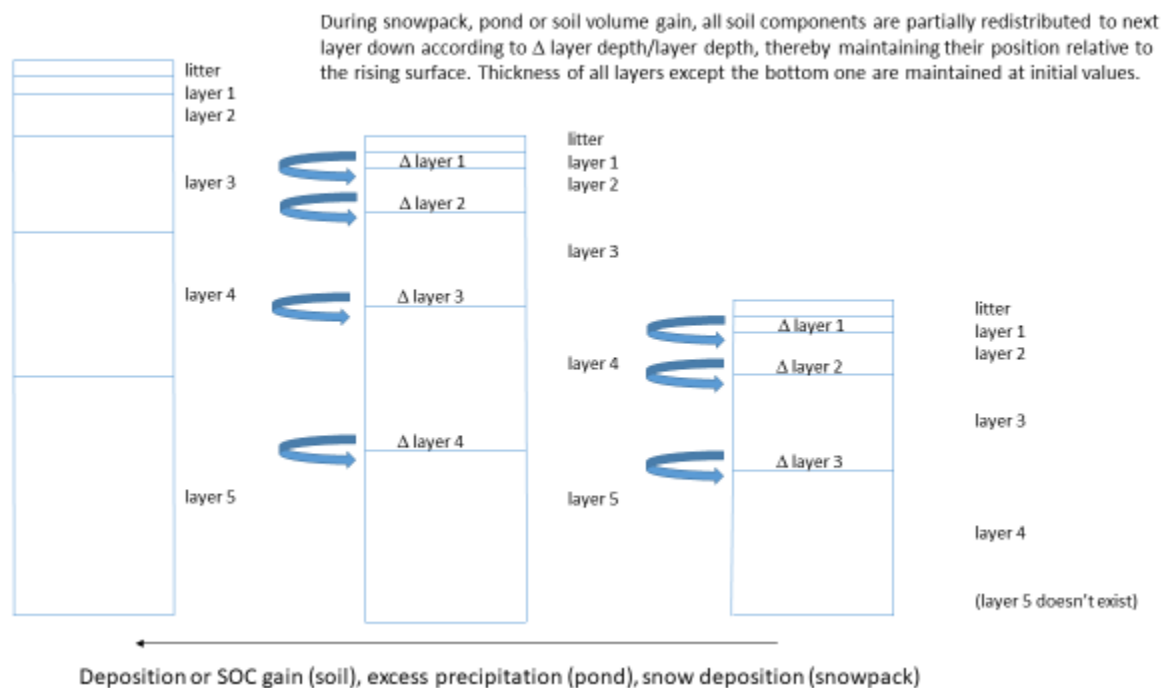
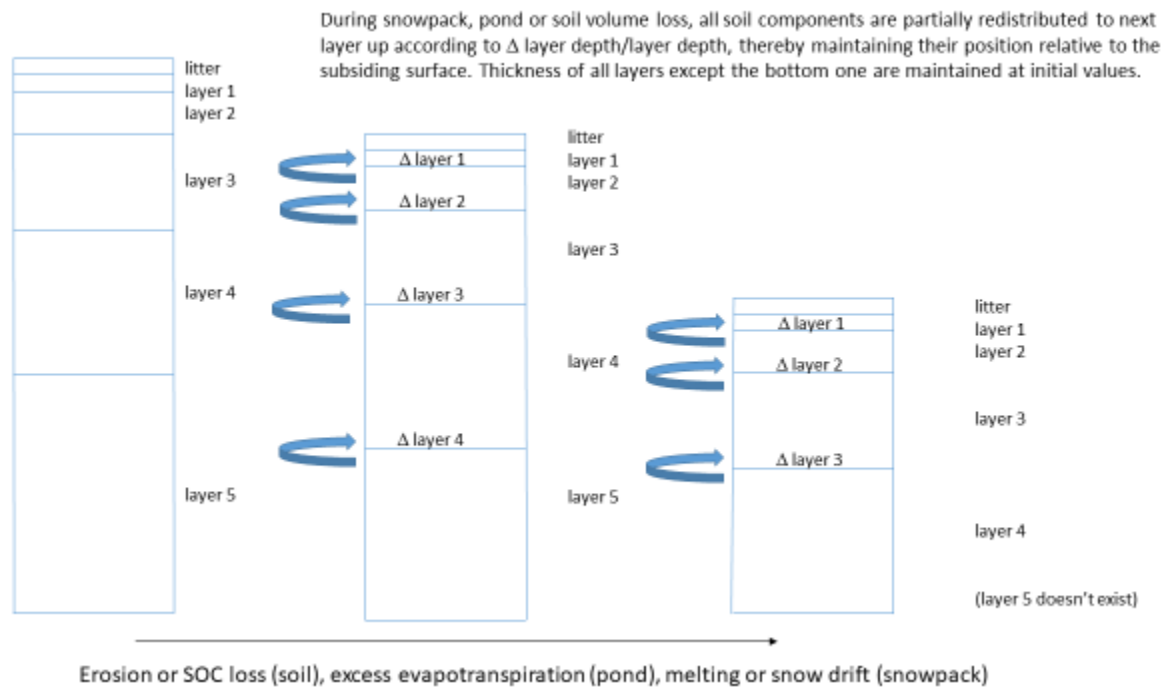


Fig. 3. Soil relayering during losses or gains in soil volumes from changes in SOC and erosion, and in snowpacks from precipitation, melting or drift.