

SUPPLEMENTAL MATERIAL

Model Development

General

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

Appendix A: Soil C, N and P Transformations

Decomposition

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

all complexes are also partitioned into components of differing vulnerability to hydrolysis.

The rate at which each component of each organic state in each complex is hydrolyzed during decomposition is a first-order function of the active biomass M of all heterotrophic microbial populations [A1,A2]. The rate at which each component is hydrolyzed is also a Monod function of substrate concentration [A3,A5], calculated from the fraction of substrate mass colonized by M [A4]. Hydrolysis rates are controlled by T_s through an Arrhenius function [A6] and by soil water content (θ) through its effect on aqueous microbial concentrations [M] [A3,A5] in surface litter and in a spatially resolved soil profile. T_s and θ are calculated from surface energy balances and from heat and water transfer schemes through canopy–snow–residue–soil profiles as described in *Energy Exchange* above. Release of N and P from hydrolysis of each component in each complex is determined by its N and P concentrations [A7] which are determined from those of the originating litterfall as described in *Autotrophic Respiration and Growth* above. Most non-lignin hydrolysis products are released as dissolved organic C, N and P (DOC, DON, and DOP) which are adsorbed or desorbed according to a power function of their soluble concentrations [A8 – A10].

Microbial Growth

The DOC decomposition product is the substrate for heterotrophic respiration (R_h) by all M in each substrate-microbe complex [A13]. Total R_h for all soil layers [A11] drives CO₂ emission from the soil surface through volatilization and diffusion. R_h may be constrained by microbial N or P concentrations, T_s , DOC and O₂ [A12 - A14]. O₂ uptake by M is driven by R_h [A16] and constrained by O₂ diffusivity to microbial surfaces [A17], as described for roots in *Autotrophic Respiration and Growth* above. Thus R_h is coupled to O₂ reduction by all aerobic M according to O₂ availability. R_h not coupled with O₂ reduction is coupled with the sequential reduction of NO₃⁻, NO₂⁻, and N₂O by heterotrophic denitrifiers, and with the reduction of organic C by fermenters and acetotrophic methanogens. In addition, autotrophic nitrifiers conduct NH₄⁺ and NO₂⁻

oxidation, and NO_2^- reduction, and autotrophic methanogens and methanotrophs conduct CH_4 production and oxidation.

All microbial populations undergo maintenance respiration R_m [A18,A19], depending on microbial N and T_s as described earlier for plants. R_h in excess of R_m is used in growth respiration R_g [A20], the energy yield ΔG of which drives growth in biomass M from DOC uptake according to the energy requirements of biosynthesis [A21, A22]. R_m in excess of R_h causes microbial dieback. M also undergoes first-order decomposition D_m [A23]. Internal retention and recycling of microbial N and P during decomposition [A24] is modelled whenever these nutrients constrain R_h [A12]. Changes in M arise from differences between gains from DOC uptake and losses from $R_m + R_g + D_m$ [A25].

Microbial Nutrient Exchange

During these changes, all microbial populations seek to maintain set minimum ratios of C:N or C:P in M by mineralizing or immobilizing NH_4^+ , NO_3^- , and H_2PO_4^- [A26], thereby controlling solution $[\text{NH}_4^+]$, $[\text{NO}_3^-]$ and $[\text{H}_2\text{PO}_4^-]$ that determine root and mycorrhizal uptake in *Nutrient Uptake and Translocation* above. If immobilization is inadequate to maintain these minimum ratios, then biomass C:N or C:P may rise, but R_h is constrained by N or P present in the lowest concentration with respect to that at the minimum ratio [A12]. Non-symbiotic heterotrophic diazotrophs can also fix aqueous N_2 [A27] to the extent that immobilization is inadequate to maintain their set minimum C:N, but at an additional respiration cost [A28]. Changes in microbial N and P arise from DON and DOP uptake plus NH_4^+ , NO_3^- , and H_2PO_4^- immobilization and N_2 fixation, less NH_4^+ , NO_3^- , and H_2PO_4^- mineralization and microbial N and P decomposition [A29].

Humification

C, N and P decomposition products in each organic matter–microbe complex are gradually stabilized into more recalcitrant organic forms with lower C:N and C:P ratios. Products from lignin hydrolysis [A1,A7] combine with some of the products from protein

and carbohydrate hydrolysis in the litterfall and manure complexes and are transferred to the POM complex [A31–A34]. Microbial decomposition products [A23, A24] from all complexes are partitioned between the humus complex and microbial residues in the originating complex according to soil clay content [A35, A36].

Appendix B: Soil-Plant Water Relations

Canopy Transpiration

Canopy energy exchange in *ecosys* is calculated from an hourly two-stage convergence solution for the transfer of water and heat through a multi-layered multi-population soil-root-canopy system. The first stage of this solution requires convergence to a value of canopy temperature T_c for each plant population at which the first-order closure of the canopy energy balance (net radiation R_n , latent heat flux LE [B1a,b], sensible heat flux H [B1c], and change in heat storage G) is achieved. These fluxes are controlled by aerodynamic (r_a) [B3] and canopy stomatal (r_c) [B2] resistances. Two controlling mechanisms are postulated for r_c which are solved in two successive steps:

- (1) At the leaf level, leaf resistance r_l [C4] controls gaseous 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 (ψ_c) (V_c'). This ratio will be allowed to vary diurnally as described in *Gross Primary Productivity* below when ψ_c is solved in the second stage of the convergence solution, described under *Water Relations* below. Values of r_{lmin} are aggregated by leaf surface area to a canopy value r_{cmin} for use in the energy balance convergence scheme [B2a].
- (2) At the canopy level, r_c rises from r_{cmin} at zero ψ_c from step (1) above through an exponential function of canopy turgor potential ψ_t [B2b] calculated from ψ_c and

osmotic water potential ψ_{π} [B4] during convergence for transpiration vs. water uptake.

Root and Mycorrhizal Water Uptake

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

Canopy Water Potential

After convergence for T_c is achieved, the difference between canopy transpiration E_c from the energy balance [B1] and total root water uptake U_c [B5] from all rooted layers in the soil is tested against the difference between canopy water content from the previous hour and that from the current hour [B14]. This difference is minimized in each iteration by adjusting ψ_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 ψ_c during convergence.

Appendix C: Gross Primary Productivity and Autotrophic Respiration

C₃ Gross Primary Productivity

After successful convergence for T_c and ψ_c (described in *Plant Water Relations* above), V_c is recalculated from that under zero ψ_c (V_c') to that under ambient ψ_c . This recalculation is driven by stomatal effects on V_g [C2] from the increase in r_{\min} at zero ψ_c [C5] to r_c at ambient ψ_c [C4], and by non-stomatal effects f_{ψ} [C9] on CO₂- and light-limited carboxylation V_b [C6] and V_j [C7] (Grant and Flanagan, 2007). The recalculation of V_c is accomplished through a convergence solution for C_i and its aqueous counterpart

C_c at which V_g [C2] equals V_c [C3] (Grant and Flanagan, 2007). The CO_2 fixation rate of each leaf surface at convergence is added to arrive at a value for gross primary productivity (GPP) by each plant population in the model [C1]. The CO_2 fixation product is stored in nonstructural C pools σ_C in each branch.

GPP is strongly controlled by nutrient uptake U_{NH_4} , U_{NO_3} and U_{PO_4} [C23], products of which are added to nonstructural N (σ_N) and P (σ_P) in root and mycorrhizal layers where they are coupled with σ_C to drive growth of branches, roots and mycorrhizae as described in *Growth and Senescence* below. Low $\sigma_N:\sigma_C$ or $\sigma_P:\sigma_C$ in branches indicate excess CO_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 CO_2 fixation by leaf σ_C accumulation widely reported in the literature.
- (2) They reduce the structural N:C and P:C ratios at which leaves are formed because σ_C , σ_N and σ_P are the substrates for leaf growth. Lower structural ratios cause a proportional reduction in areal concentrations of rubisco [C6b] and chlorophyll [C7b], reducing leaf CO_2 fixation.

Autotrophic Respiration

The temperature-dependent oxidation of these nonstructural pools (R_c) [C14], plus the energy costs of nutrient uptake [C23], drive autotrophic respiration (R_a) [C13] by all branches, roots and mycorrhizae. R_c by roots and mycorrhizae is constrained by O_2 uptake U_{O_2} [C14b] calculated by solving for aqueous O_2 concentrations at root and mycorrhizal surfaces [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 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 O_2 concentrations sustained by transport and dissolution of gaseous O_2 through soil and roots (Grant 2004), and are governed by lengths and surface areas of roots and mycorrhizae (Grant, 1998).

Thus R_c is coupled to O_2 reduction by all root and mycorrhizal populations according to O_2 availability. R_c is first used to meet maintenance respiration requirements (R_m), calculated independently of R_c from the N content in each organ, and a function of T_c or T_s [C16]. Any excess of R_c over R_m is expended as growth respiration R_g , constrained by branch, root or mycorrhizal ψ_t [C17]. When R_m exceeds R_c , the shortfall is met by the respiration of remobilizable C (R_s) in leaves and twigs or roots and mycorrhizae [C15].

Growth and Senescence

R_g drives the conversion of branch σ_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 σ_C into primary and secondary axes according to root and mycorrhizal growth yields. Growth also requires organ-specific ratios of nonstructural N (σ_N) and P (σ_P) from U_{NH_4} , U_{NO_3} and U_{PO_4} [C23] which are coupled with σ_C to drive growth of branches, roots and mycorrhizae.

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

σ_P from root to branch and slow transfer of σ_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 σ_C , σ_N and σ_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 ψ_t [C17], and because branch ψ_t declines relatively more with soil drying than does root ψ_t , branch R_g also declines relatively more with soil drying than does root R_g , slowing oxidation of σ_C in branches and allowing more translocation of σ_C from branches to roots. This change in allocation of σ_C enables more root growth to reduce Ω_s , Ω_t and Ω_a , and hence increase U [B6], thereby offsetting the effects of soil drying on ψ_t . Thus the modelled plant translocates σ_C , σ_N and σ_P among branches, roots and mycorrhizae to maintain a functional equilibrium between acquisition and use of water.

R_s [C15] drives the withdrawal of remobilizable C, N and P (mostly nonstructural protein) from leaves and twigs or roots and mycorrhizae into σ_N and σ_P , and the loss of associated non-remobilizable C, N and P (mostly structural) as litterfall [C18]. Provision is also made to withdraw remobilizable N or P from leaves and twigs or roots and mycorrhizae when ratios of $\sigma_N:\sigma_C$ or $\sigma_P:\sigma_C$ become smaller than those required for growth of new phytomass. This withdrawal drives the withdrawal of associated remobilizable C, and the loss of associated non-remobilizable C, N and P as litterfall. Environmental constraints such as water, heat, nutrient or O_2 stress that reduce σ_C and hence R_c with respect to R_m therefore hasten litterfall.

R_a of each branch or root and mycorrhizal layer is the total of R_c and R_s , and net primary productivity (NPP) is the difference between canopy GPP [C1] and total R_a of all branches and root and mycorrhizal layers [C13]. Phytomass net growth is the difference between gains driven by R_g and Y_g , and losses driven by R_s and litterfall [C20]. These gains are allocated to leaves, twigs, wood and reproductive material at successive branch

nodes, and to roots and mycorrhizae at successive primary and secondary axes, driving leaf expansion [C21a] and root extension [C21b]. Losses from remobilization and litterfall in shoots start at the lowest node of each branch at which leaves or twigs are present, and proceed upwards when leaves or twigs are lost. Losses in roots and mycorrhizae start with secondary axes and proceeds to primary axes when secondary axes are lost.

Root and Mycorrhizal Nutrient Uptake

Root and mycorrhizal uptake of N and P U_{NH_4} , U_{NO_3} and U_{PO_4} is calculated by solving for solution $[\text{NH}_4^+]$, $[\text{NO}_3^-]$ and $[\text{H}_2\text{PO}_4^-]$ at root and mycorrhizal surfaces at which radial transport by mass flow and diffusion from the soil solution to these surfaces [C23a,c,e] equals active uptake by the surfaces [C23b,d,f]. Path lengths and surface areas for U_{NH_4} , U_{NO_3} and U_{PO_4} are calculated from a root and mycorrhizal growth submodel driven by exchange of nonstructural C, N and P along concentration gradients generated by uptake vs. consumption of C, N and P in shoots and roots (Grant, 1998). A product inhibition function is included to avoid uptake in excess of nutrient requirements [C23g].

C₄ Gross Primary Productivity

C₄ Mesophyll

In C₄ plants, the mesophyll carboxylation rate is the lesser of CO₂- and light-limited reaction rates [C26] (Berry and Farquhar, 1978). The CO₂-limited rate is a Michaelis-Menten function of PEP carboxylase (PEPc) activity and aqueous CO₂ 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 C₄ product inhibition (Jiao and Chollet, 1988; Lawlor, 1993) [C34], ψ_c ([C35] as described in Grant and Flanagan, 2007) and T_c [C36]. 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. CO₂ fixation.

C₄ Mesophyll-Bundle Sheath Exchange

Differences in the mesophyll and bundle sheath concentrations of the C₄ carboxylation product drive mesophyll-bundle sheath transfer (Leegood, 2000) [C37]. The bundle sheath concentration of the C₄ product drives a product-inhibited decarboxylation reaction (Laisk and Edwards, 2000) [C38], the CO₂ product of which generates a concentration gradient that drives leakage of CO₂ from the bundle sheath to the mesophyll [C39]. CO₂ in the bundle sheath is maintained in 1:50 equilibrium with HCO₃⁻ (Laisk and Edwards, 2000). At this stage of model development, the return of a C₃ 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 C₄ carboxylation products from [C40 – C41] to be maintained at values consistent with those in Leegood (2000), bundle sheath concentrations of CO₂ (from Eq. [C42]) to be maintained at values similar to those reported by Furbank and Hatch (1987), and bundle sheath CO₂ 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).

C₄ Bundle Sheath

A C₃ model in which carboxylation is the lesser of CO₂- and light-limited reaction rates (Farquhar et al., 1980) has been parameterized for the bundle sheath of C₄ plants [C43] from Seeman et al. (1984). The CO₂-limited rate [C44] is a Michaelis-Menten function of RuBP carboxylase (RuBPc) activity and bundle sheath CO₂ concentration [C42]. The light-limited rate [C45] 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 C₃ product inhibition (Bowes, 1991; Stitt, 1991) [C49], ψ_c (Eq. A12 from Grant and Flanagan, 2007) and T_c [C36].

Rates of C₃ product removal are controlled by phytomass biosynthesis rates driven by concentrations of nonstructural products from leaf CO₂ 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 C₃ carboxylation [C43], raise bundle sheath CO₂ concentration [C42], accelerate CO₂ leakage [C39], slow C₄ decarboxylation [C38], raise C₄ product concentration in the bundle sheath [C41], slow C₄ product transfer from the mesophyll [C37], raise C₄ product concentration in the mesophyll [C40], and slow mesophyll CO₂ fixation [C32 – C35]. This reaction sequence simulates the progressive inhibition of C₃ and C₄ carboxylation hypothesized by Sawada et al. (2002) following partial removal of C sinks in C₄ plants.

Appendix D: Soil Water, Heat, Gas and Solute Fluxes

Surface Water Flux

Surface runoff is modelled using Manning's equation [D1] with surface water velocity v [D3] calculated from surface geometry [D5a] and slope [D5b], and with surface water depth d [D2] calculated from surface water balance [D4] using kinematic wave theory.

Subsurface Water Flux

Subsurface water flow [D7] is calculated from Richard's equation using bulk soil water potentials ψ_s of both cells if both source and destination cells are unsaturated [D9a], or Green-Ampt equation using ψ_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.

Exchange with Water Table

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

Surface Heat Flux

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

Gas Flux

All gases undergo volatilization – dissolution between the gaseous and aqueous phases in the soil [D14a] and root [D14b], and between the atmosphere and the aqueous phase at the soil surface [D15a], driven by gaseous – aqueous concentration differences calculated from solubility coefficients and coupled to diffusive uptake by roots [C14] and microbes [A17]. Gases also undergo convective - conductive transfer among soil layers driven by gaseous concentration gradients and diffusivities [D16a,b,c] calculated from air-filled porosities [D17a,b,c], and from each rooted soil layer directly to the atmosphere through roots driven by gaseous concentration gradients and diffusivities [D16d] calculated from root porosities [D17d]. Gases may also bubble upwards from soil zones in which the total partial pressure of all aqueous gases exceeds atmospheric pressure [D18].

Solute Flux

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

Appendix E: Solute Transformations

Precipitation - Dissolution Equilibria

Solution $[\text{NH}_4^+]$, $[\text{NO}_3^-]$ and $[\text{H}_2\text{PO}_4^-]$ that drive U_{NH_4} , U_{NO_3} and U_{PO_4} [C23] are controlled by precipitation, adsorption and ion pairing reactions (Grant et al., 2004; Grant and Heaney, 1997), including precipitation-dissolution of $\text{Al}(\text{OH})_3$, $\text{Fe}(\text{OH})_3$, CaCO_3 , CaSO_4 , AlPO_4 , FePO_4 , $\text{Ca}(\text{H}_2\text{PO}_4)_2$, CaHPO_4 , and $\text{Ca}_5(\text{PO}_4)_3\text{OH}$ [E1 – E9], cation exchange between Ca^{2+} , NH_4^+ and other cations [E10 – E15], anion exchange between adsorbed and soluble H_2PO_4^- , HPO_4^{2-} and OH^- [E16 – E20], and ion pairing [E22 – E55].

Key governing equations for simulating net ecosystem productivity in *ecosys*. Variables input to the model appear in bold with values given in the **Definition of Variables** below.

Appendix F: N₂ Fixation

Rhizobial Growth

Modelling the activity of symbiotic N₂ fixing bacteria in roots follows a protocol similar to that of non-symbiotic N₂ fixing bacteria in soil. Respiration demand is driven by specific activity, microbial biomass M_n , and nonstructural C concentration $[\chi_n]$ in root nodules [F1], and is constrained by temperature [F2] and microbial N or P status [F3]. Nodule respiration R is constrained by the extent to which O₂ uptake meets O₂ demand [F4] imposed by respiration demand [F5]. O₂ uptake is in turn constrained by rhizosphere $[\text{O}_{2r}]$ [F6a] which is controlled by radial diffusion of O₂ through soil water to roots and

nodules [F6b]. Soil water $[O_2]$ is maintained by dissolution of O_2 from soil air which is in turn maintained by soil-atmosphere gas exchange and vertical diffusion (Grant, 2004). R_h is first allocated to maintenance respiration R_m [F7 – F8] and the remainder if any is allocated to growth respiration R_g [F9]. If R_m exceeds R_h , the shortfall is made up from respiration of microbial protein C, forcing senescence and litterfall of associated non-protein C [F10 – F11].

N₂ Fixation

N_2 fixation V_{N_2} is driven by R_g [F12], but is constrained by accumulation of nonstructural N v_n with respect to nonstructural C and P also required for microbial growth in the nodule [F13]. Nonstructural N v_{nd} is the product of V_{N_2} , so that [F12] simulates the inhibition of N_2 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_2 fixation is constrained by the need of nodule bacteria for N not met from other sources (Postgate, 1998). Respiration required for N_2 fixation R_{N_2} [F14] is subtracted from R_g [F15] when calculating microbial growth [F16 – F18]. Microbial senescence drives N and P litterfall [F19 – F20].

Nodule – Root Exchange

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

Root nonstructural N (ν_r) may rise if high mineral N concentrations in soil sustain rapid N uptake by roots. Large ν_r suppresses or even reverses the transfer of ν_n from nodule to root [F22], raising ν_n [F25] and hence suppressing V_{N_2} [F12 – F13]. Large ν_r also accelerates the consumption of χ_r , slowing its transfer to nodules [F21], reducing χ_n [F24] and hence slowing nodule growth [F1]. Conversely, slow root N uptake caused by low soil mineral N concentrations would lower ν_{rt} and raise χ_{rt} , hastening the transfer of ν_n from nodule to root and of χ_{rt} from root to nodule, lowering ν_n , raising χ_n , and accelerating V_{N_2} . However [F13] also allows V_{N_2} to be constrained by nonstructural C and P concentrations arising from CO_2 fixation and root P uptake.

Appendix A: Soil C, N and P Transformations

Decomposition

$D_{Si,j,l,C} = D'_{Si,j,l,C} \sum_n M_{i,n,a,l,C} f_{igl}$	decomposition of litter, SOC	[A1]
$D_{Zi,j,l,C} = D'_{Zi,j,l,C} \sum_n M_{i,n,a,l,C} f_{igl}$	decomposition of microbial residues	[A2]
$D'_{Si,j,l,C} = \{D_{Sj,C}[S_{i,j,l,C}]\} / \{[S_{i,j,l,C}] + K_{mD}(1.0 + [\sum_n M_{i,n,a,l,C}]/K_{iD})\}$	substrate and water constraint on D from colonized substrate mass	[A3]
$\delta S_{i,j,k,l,C} / \delta t = \beta \sum_n (U_{i,n,l,C} - R_{hi,n,l}) (S'_{i,j,k,l,C} / S'_{i,j,l,C}) \{ (S'_{i,j,l,C} / S_{i,j,l,C}) / (S'_{i,j,l,C} / S_{i,j,l,C} + K_{iS}) \}$	substrate mass determined by microbial growth into uncolonized substrate mass	[A4]
$D'_{Zi,j,l,C} = \{D_{Zj,C}[Z_{i,j,l,C}]\} / \{[Z_{i,j,l,C}] + K_{mD}(1.0 + [\sum_n M_{i,n,a,l,C}]/K_{iD})\}$	substrate and water constraint on D from microbial residues	[A5]
$f_{igl} = T_{sl} \{ e^{[B - H_a / (RT_{sl})]} \} / \{ 1 + e^{[(H_{dl} - ST_{sl}) / (RT_{sl})]} + e^{[(ST_{sl} - H_{dh}) / (RT_{sl})]} \}$	Arrhenius function for D and R_h	[A6]
$D_{Si,j,l,N,P} = D_{Si,j,l,C} (S_{i,j,l,N,P} / S_{i,j,l,C})$	N and P coupled with C during D	[A7a]
$D_{Zi,j,l,N,P} = D_{Zi,j,l,C} (Z_{i,j,l,N,P} / Z_{i,j,l,C})$		[A7b]
$Y_{i,l,C} = k_{ts} (aF_s [Q_{i,l,C}]^b - X_{i,l,C})$	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]
$Y_{i,l,N,P} = Y_{i,l,C} (X_{i,l,N,P} / X_{i,l,C})$	$(Y_{i,l,C} < 0)$ desorption of DON, DOP	[A10]

Microbial Growth

$R_h = \sum_i \sum_n \sum_l R_{hi,n,l}$		[A11]
$R_{hi,n,l} = R'_{hn} \min\{C_{Ni,n,l,a} / C_{Nj}, C_{Pi,n,l,a} / C_{Pj}\}$	R_h constrained by microbial N, P	[A12]
$R'_{i,n,l} = M_{i,n,a,l,C} \{R_{hi,n,l} [Q_{i,l,C}]\} / \{ (K_{mQC} + [Q_{i,l,C}]) \} f_{igl} f_{vgl}$	R_h constrained by substrate DOC	[A13]

$$R_{hi,n,l} = R_{h',i,n,l} (U_{O2i,n,l} / U'_{O2i,n,l}) \quad R_h \text{ constrained by } O_2 \quad [A14]$$

$$f_{\psi_{gl}} = 1.0 - 6.67(1.0 - e^{(M\psi_s/(RT_s l)}) \quad \psi_s \text{ constraints on microbial growth} \quad [A15]$$

$$U'_{O2i,n,l} = 2.67R_{h',i,n,l} \quad O_2 \text{ demand driven by potential } R_h \quad [A16]$$

$$U_{O2i,n,l} = U'_{O2i,n,l} [O_{2mi,n,l}] / ([O_{2mi,n,l}] + K_{O_2}) \quad \text{active uptake coupled with radial diffusion of } O_2 \quad [A17a]$$

$$= 4\pi n M_{i,n,a,l,C} D_{sO_2} [r_m r_{wl} / (r_{wl} - r_m)] ([O_{2sl}] - [O_{2mi,n,l}]) \quad [A17b]$$

$$R_{mi,n,j,l} = R_m M_{i,n,j,l,N} f_{uml} \quad [A18]$$

$$f_{uml} = e^{[y(T_{sl} - 298.16)]} \quad [A19]$$

$$R_{gi,n,l} = R_{hi,n,l} - \sum_j R_{mi,n,j,l} \quad [A20]$$

$$U_{i,n,l,C} = \min(R_{hi,n,l}, \sum_j R_{mi,n,j,l}) + R_{gi,n,l} (1 + \Delta G/E_m) \quad \text{DOC uptake driven by } R_g \quad [A21]$$

$$U_{i,n,l,N,P} = U_{i,n,l} Q_{i,l,N,P} / Q_{i,l,C} \quad \text{DON,DOP uptake driven by } U_{i,n,l,C} \quad [A22]$$

$$D_{Mi,n,j,l,C} = D_{Mij} M_{i,n,j,C} f_{ig} \quad \text{first-order decay of microbial C,} \quad [A23]$$

$$D_{Mi,n,j,l,N,P} = D_{Mij} M_{i,n,j,l,N,P} f_{ig} f_{di,n,l,N,P} \quad \text{partial release of microbial N, P} \quad [A24]$$

$$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,l,C} - F_j R_{hi,n,l} - D_{Mi,n,j,l,C} \quad [R_{hi,n,l} > R_{mi,n,j,l}] \quad \text{growth} \quad [A25a]$$

$$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,l,C} - R_{mi,n,j,l} - D_{Mi,n,j,l,C} \quad [R_{hi,n,l} < R_{mi,n,j,l}] \quad \text{senescence} \quad [A25b]$$

Microbial Nutrient Exchange

$$U_{NH_4i,n,j,l} = (M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N}) \quad U_{NH_4} < 0 \quad \text{mineralization} \quad [A26a]$$

$$U_{NH_4i,n,j,l} = \min\{ (M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N}), \quad U'_{NH_4} A_{i,n,j,l} ([NH_4^+_{i,n,j,l}] - [NH_4^+_{mn}]) / ([NH_4^+_{i,n,j,l}] - [NH_4^+_{mn}] + K_{NH_4}) \} \quad U_{NH_4} > 0 \quad \text{immobilization} \quad [A26b]$$

$$U_{NO_3i,n,j,l} = \min\{ (M_{i,n,j,l,C} C_{Nj} - (M_{i,n,j,l,N} + U_{NH_4i,n,j,l})), \quad U'_{NO_3} A_{i,n,j,l} ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}]) / ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}] + K_{NO_3}) \} \quad U_{NO_3} > 0 \quad \text{immobilization} \quad [A26c]$$

$$U_{\text{PO}_4 i,n,j,l} = (M_{i,n,j,l,C} C_{\text{Pj}} - M_{i,n,j,l,P})$$

$$U_{\text{PO}_4} < 0 \quad \text{mineralization} \quad [\text{A26d}]$$

$$U_{\text{PO}_4 i,n,j,l} = \min\{(M_{i,n,j,l,C} C_{\text{Pj}} - M_{i,n,j,l,P}), \\ U'_{\text{PO}_4} A_{i,n,j,l} ([\text{H}_2\text{PO}_4^-]_{i,n,j,l} - [\text{H}_2\text{PO}_4^-]_{\text{mn}}) / ([\text{H}_2\text{PO}_4^-]_{i,n,j,l} - [\text{H}_2\text{PO}_4^-]_{\text{mn}} + K_{\text{PO}_4})\}$$

$$U_{\text{PO}_4} > 0 \quad \text{immobilization} \quad [\text{A26e}]$$

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

$$\text{N}_2 \text{ fixation driven by N deficit of} \\ \text{diazotrophic population} \quad [\text{A27}]$$

$$R_{\Phi i,n=f,j,l} = E_{\Phi} \Phi_{i,n=f,j,l}$$

$$[\text{A28}]$$

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

$$\text{growth vs. losses of microbial N, P} \quad [\text{A29a}]$$

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

$$[\text{A29b}]$$

$$M_{i,n,a,l,C} = M_{i,n,j=\text{labile},l,C} + M_{i,n,j=\text{resistant},l,C} F_r / F_1$$

$$[\text{A30}]$$

Humification

$$H_{S_{i,j=\text{lignin}},l,C} = D_{S_{i,j=\text{lignin}},l,C}$$

$$\text{decomposition products of litter} \\ \text{added to POC depending on lignin} \quad [\text{A31}]$$

$$H_{S_{i,j=\text{lignin}},l,N,P} = D_{S_{i,j=\text{lignin}},l,N,P}$$

$$[\text{A32}]$$

$$H_{S_{i,j \neq \text{lignin}},l,C} = H_{S_{i,j=\text{lignin}},l,C} L_{\text{hj}}$$

$$[\text{A33}]$$

$$H_{S_{i,j \neq \text{lignin}},l,N,P} = H_{S_{i,j=\text{lignin}},l,C} S_{i,l,N,P} / S_{i,l,C}$$

$$[\text{A34}]$$

$$H_{M_{i,n,j,l,C}} = D_{M_{i,n,j,l,C}} F_{\text{h}}$$

$$\text{decomposition products of} \\ \text{microbes added to humus} \quad [\text{A35}]$$

$$H_{M_{i,n,j,l,N,P}} = H_{M_{i,n,j,l,C}} M_{i,n,j,l,N,P} / M_{i,n,j,l,C}$$

$$\text{depending on clay} \quad [\text{A36}]$$

Definition of Variables in Appendix A

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus				
<i>j</i>	kinetic component: labile, resistant, active				
<i>l</i>	soil or litter layer				
<i>n</i>	microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)				
<i>variables</i>					
<i>A</i>	microbial surface area	$\text{m}^2 \text{ m}^{-2}$	[A26]		
<i>a</i>	total substrate + residue C = ($[S_{i,j,C}] + [Z_{i,j,C}]$)	g C Mg^{-1}	[A8]		
<i>B</i>	parameter such that $f_{\text{ig}} = 1.0$ at $T_l = 298.15 \text{ K}$		[A6]	26.230	
<i>b</i>	Freundlich exponent for sorption isotherm		[A8]	0.85	Grant et al. (1993a,b)
β	specific colonization rate of uncolonized substrate	-	[A4]	5.0	Grant et al. (2010)
$C_{N,Pi,n,a,l}$	ratio of $M_{i,n,a,N,P}$ to $M_{i,n,a,C}$	g N or P g C^{-1}	[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^{-1}	[A12,A26,A27]	0.22 and 0.13 (N), 0.022 and 0.013 (P) for $j = \text{labile}$ and resistant, respectively	Grant et al. (1993a,b)

$D_{Mi,j}$	specific decomposition rate of $M_{i,n,j}$ at 30°C	$\text{g C g C}^{-1} \text{h}^{-1}$	[A23,A24]	0.0125 and 0.00035 for $j =$ labile and resistant, respectively	Grant et al. (1993a,b)
$D_{Mi,n,j,l,C}$	decomposition rate of $M_{i,n,j,l,C}$	$\text{g C m}^{-2} \text{h}^{-1}$	[A23,A25,A35]		
$D_{Mi,n,j,l,N,P}$	decomposition rate of $M_{i,n,j,l,N,P}$	$\text{g N or P m}^{-2} \text{h}^{-1}$	[A24,A29]		
D_{sO_2l}	aqueous dispersivity–diffusivity of O_2 during microbial uptake in soil	$\text{m}^2 \text{h}^{-1}$	[A17]		
$D_{Si,j,l,C}$	decomposition rate of $S_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ producing Q in [A13]	$\text{g C m}^{-2} \text{h}^{-1}$	[A1,A7a,A31]		
$D_{Sj,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ at 25°C and saturating[$S_{i,l,C}$]	$\text{g C g C}^{-1} \text{h}^{-1}$	[A3]	1.0, 1.0, 0.15, and 0.025 for $j =$ protein, carbohydrate, cellulose, and lignin	Grant et al. (1993a,b)
$D_{Si,j,l,N,P}$	decomposition rate of $S_{i,j,l,N,P}$ by $\sum_n M_{i,n,a,l}$	$\text{g N or P m}^{-2} \text{h}^{-1}$	[A7a, A32]		
$D_{Zi,j,l,C}$	decomposition rate of $Z_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ producing Q in [A13]	$\text{g C m}^{-2} \text{h}^{-1}$	[A2,A7b]		
$D_{Zi,j,N,P}$	decomposition rate of $Z_{i,j,l,N,P}$ by $\sum_n M_{i,n,a,l}$	$\text{g N or P m}^{-2} \text{h}^{-1}$	[A7b]		
$D_{Zj,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ at 25°C and saturating[$Z_{i,l,C}$]	$\text{g C g C}^{-1} \text{h}^{-1}$	[A5]	0.25 and 0.05 for $j =$ labile and resistant biomass	Grant et al. (1993a,b)
$D'_{Si,j,l,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ at 25°C	$\text{g C g C}^{-1} \text{h}^{-1}$	[A1,A3]		
$D'_{Zi,j,l,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\sum_n M_{i,n,a,l}$ at 25°C	$\text{g C g C}^{-1} \text{h}^{-1}$	[A2,A5]		
ΔG	energy yield of C oxidation and O_2 reduction	kJ g C^{-1}	[A21]	37.5	
E_m	energy requirement for growth of $M_{i,n,a,l}$	kJ g C^{-1}	[A21]	25	

E_{ϕ}	energy requirement for non-symbiotic N ₂ fixation by heterotrophic diazotrophs ($n = f$)	g C g N ⁻¹	[A28]	5	Waring and Running (1998)
F_h	fraction of products from microbial decomposition that are humified (function of clay content)		[A35]	0.167 + 0.167*clay	
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]		
$f_{\text{ai},n,\text{N,P}}$	fraction of N or P released with $D_{Mi,n,j,l,C}$ during decomposition	dimensionless	[A24]	0.33 $U_{\text{NH}_4} > 0$ 1.00 $U_{\text{NH}_4} < 0$ 0.33 $U_{\text{PO}_4} > 0$ 1.00 $U_{\text{PO}_4} < 0$	
f_{tgl}	temperature function for microbial growth respiration	dimensionless	[A1,A2,A6,A13,A23,A24]		
f_{tml}	temperature function for maintenance respiration	dimensionless	[A18,A19]		
f_{vgl}	soil water potential function for microbial, root or mycorrhizal growth respiration	dimensionless	[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	[A27,A28,A29]		
[H ₂ PO ₄ ⁻]	concentration of H ₂ PO ₄ ⁻ in soil solution	g P m ⁻³	[A26]		
H_a	energy of activation	J mol ⁻¹	[A6,C10]	65 x 10 ³	Addiscott (1983)
H_{dh}	energy of high temperature deactivation	J mol ⁻¹	[A6,C10]	225 x 10 ³	
H_{dl}	energy of low temperature deactivation	J mol ⁻¹	[A6,C10]	198 x 10 ³	
$H_{Mi,n,j,l,C}$	transfer of microbial C decomposition products to humus	g C m m ⁻² h ⁻¹	[A35,A36]		
$H_{Mi,n,j,l,\text{N,P}}$	transfer of microbial N or P decomposition products to humus	g N or P m ⁻² h ⁻¹	[A36]		
$H_{Si,j,l,C}$	transfer of C hydrolysis products to particulate OM	g C m ⁻² h ⁻¹	[A31,A32,A33,A34]		

$H_{Si,j,l,N,P}$	transfer of N or P hydrolysis products to particulate OM	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A32,A34]		
K_{iS}	inhibition constant for microbial colonization of substrate	-	[A4]	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 $[M_{i,n,a}]$ on $S_{i,C}$, $Z_{i,C}$	g C m^{-3}	[A3,A5]	25	Grant et al. (1993a,b); Lizama and Suzuki (1990)
K_{mD}	Michaelis–Menten constant for $D_{Si,j,C}$	g C Mg^{-1}	[A3,A5]	75	
K_{mQ_C}	Michaelis–Menten constant for $R'_{hi,n}$ on $[Q_{i,C}]$	g C m^{-3}	[A13]	36	
K_{O_2}	Michaelis–Menten constant for reduction of O_2 by microbes, roots and mycorrhizae	$\text{g O}_2 \text{ m}^{-3}$	[A17]	0.064	Griffin (1972)
k_{is}	equilibrium rate constant for sorption	h^{-1}	[A8]	0.01	Grant et al. (1993a,b)
L_{hj}	ratio of nonlignin to lignin components in humified hydrolysis products		[A33]	0.10, 0.05, and 0.05 for $j =$ protein, carbohydrate, and cellulose, respectively	Shulten and Schnitzer (1997)
M	molecular mass of water	g mol^{-1}	[A15]	18	
$M_{i,n,j,l,C}$	microbial C	g C m^{-2}	[A1,A2,A13,A17,A23,A25,A26,A30,A36]		
$M_{i,n,j,l,N}$	microbial N	g N m^{-2}	[A18,A27,A29]		
$M_{i,n,j,l,P}$	microbial P	g P m^{-2}	[A24,A29,A26,A36]		
$M_{i,n,a,l,C}$	active microbial C from heterotrophic population n associated with $(S_{i,j,l,C} + Z_{i,j,l,C})$	g C m^{-2}	[A1,A2,A13,A17,A30]		

$[M_{i,n,a,l,C}]$	concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,l,C} / \theta_l$	g C m^{-3}	[A3, A5]	
$[\text{NH}_4^+_{i,n,j,l}]$	concentration of NH_4^+ at microbial surfaces	g N m^{-3}	[A26]	
$[\text{NH}_4^+_{mn}]$	concentration of NH_4^+ at microbial surfaces below which $U_{\text{NH}_4} = 0$	g N m^{-3}	[A26]	0.0125
$[\text{NO}_3^-_{i,n,j,l}]$	concentration of NO_3^- at microbial surfaces	g N m^{-3}	[A26]	
$[\text{NO}_3^-_{mn}]$	concentration of NO_3^- at microbial surfaces below which $U_{\text{NO}_3} = 0$	g N m^{-3}	[A26]	0.03
$[\text{H}_2\text{PO}_4^-_{i,n,j,l}]$	concentration of H_2PO_4^- at microbial surfaces	g N m^{-3}	[A26]	
$[\text{H}_2\text{PO}_4^-_{mn}]$	concentration of H_2PO_4^- at microbial surfaces below which $U_{\text{PO}_4} = 0$	g N m^{-3}	[A26]	0.002
$[\text{O}_{2mi,n,l}]$	O_2 concentration at heterotrophic microsities	$\text{g O}_2 \text{ m}^{-3}$	[A17]	
$[\text{O}_{2sl}]$	O_2 concentration in soil solution	$\text{g O}_2 \text{ m}^{-3}$	[A17]	
$Q_{i,l,C}$	<i>DOC</i> from products of $D_{Si,j,l,C}$ [A3] and $D_{Zi,j,l,C}$ [A5]	g C m^{-2}	[A8,A13,A22]	
$[Q_{i,l,C}]$	solution concentration of $Q_{i,l,C}$	g C Mg^{-1}	[A8,A13]	
$Q_{i,l,N,P}$	<i>DON</i> and <i>DOP</i> from products of $(D_{Si,j,l,N,P} + D_{Zi,j,l,N,P})$	g N or P m^{-2}	[A9,A22]	
R	gas constant	$\text{J mol}^{-1} \text{ K}^{-1}$	[A6,A15,C10]	8.3143
$R_{\phi,n=f,j,l}$	respiration for non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	$\text{g C m}^{-2} \text{ h}^{-1}$	[A28]	
$R_{gi,n,l}$	growth respiration of $M_{i,n,a,l}$ on $Q_{i,l,C}$ under nonlimiting O_2 and nutrients	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A20]	
R_h	total heterotrophic respiration of all $M_{i,n,a,l}$ under ambient DOC , O_2 , nutrients, θ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A11]	
$R_{hi,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under ambient DOC , O_2 , nutrients, θ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A4,A11,A14,A20, A21,A25]	
$R_{hi,n,l}$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2 , DOC , θ and 25°C	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A12,A13]	

R_h'	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting DOC, O ₂ , nutrients, θ and 25°C	g C g C ⁻¹ h ⁻¹	[A12]	0.125	Shields et al. (1973)
$R_{h',i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O ₂ and ambient DOC, nutrients, θ and temperature	g C m ⁻² h ⁻¹	[A13,A14,A16]		
R_m	specific maintenance respiration at 25°C	g C g N ⁻¹ h ⁻¹	[A18]	0.0115	Barnes et al. (1998)
$R_{m,i,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	g C m ⁻² h ⁻¹	[A18,A20,A21,A25]		
r_{wl}	radius of r_m + water film at current water content	m	[A17]		
r_m	radius of heterotrophic microsite	m	[A17]	2.5×10^{-6}	
r_{wl}	thickness of water films	m	[A17]		
S	change in entropy	J mol ⁻¹ K ⁻¹	[A6,C10]	710	Sharpe and DeMichelle (1977)
$[S_{i,j,l,C}]$	concentration of $S_{i,j,l,C}$ in soil	g C Mg ⁻¹	[A3]		
$S_{i,j,l,C}$	mass of colonized solid or sorbed organic C in soil	g C m ⁻²	[A4,A7a,A33]		
$S'_{i,j,l,C}$	mass of uncolonized solid or sorbed organic C in soil	g C m ⁻²	[A4]		
$S_{i,j,l,N,P}$	mass of solid or sorbed organic N or P in soil	g N or P m ⁻²	[A7a,A33]		
T_{sl}	soil temperature	K	[A6,A15.A19]		
$U_{i,n,C}$	uptake of $Q_{i,l,C}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g C m ⁻² h ⁻¹	[A4,A21,A22,A25]		
$U_{i,n,N,P}$	uptake of $Q_{i,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g N or P m ⁻² h ⁻¹	[A22,A29]		
$U_{NH_4,i,n,j,l}$	NH ₄ ⁺ uptake by microbes	g N m ⁻² h ⁻¹	[A26, A27,A29]		
U'_{NH_4}	maximum U_{NH_4} at 25 °C and non-limiting NH ₄ ⁺	g N m ⁻² h ⁻¹	[A26]	5.0×10^{-3}	
$U_{NO_3,i,n,j,l}$	NO ₃ ⁻ uptake by microbes	g N m ⁻² h ⁻¹	[A26,A27,A29]		

U'_{NO_3}	maximum U_{NO_3} at 25 °C and non-limiting NO_3^-	$\text{g N m}^{-2} \text{h}^{-1}$	[A26]	5.0×10^{-3}
$U_{\text{O}_2i,n}$	O_2 uptake by $M_{i,n,a,l}$ under ambient O_2	$\text{g m}^{-2} \text{h}^{-1}$	[A14,A17]	
$U'_{\text{O}_2i,n}$	O_2 uptake by $M_{i,n,a,l}$ under nonlimiting O_2	$\text{g m}^{-2} \text{h}^{-1}$	[A14,A16,A17]	
$U_{\text{PO}_4i,n,j,l}$	H_2PO_4^- uptake by microbes	$\text{g N m}^{-2} \text{h}^{-1}$	[A26,A27,A29]	
U'_{PO_4}	maximum U_{PO_4} at 25 °C and non-limiting H_2PO_4^-	$\text{g N m}^{-2} \text{h}^{-1}$	[A26]	5.0×10^{-3}
$X_{i,l,C}$	adsorbed C hydrolysis products	g C Mg^{-1}	[A8,A10]	
$X_{i,l,N,P}$	adsorbed N or P hydrolysis products	g P Mg^{-1}	[A10]	
y	selected to give a Q_{10} for f_{tm} of 2.25		[A19]	0.081
ψ_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	g C Mg^{-1}	[A5]	
$Z_{i,j,l,C}$	mass of microbial residue C in soil	g C m^{-2}	[A7b]	
$Z_{i,j,l,N,P}$	mass of microbial residue P in soil	g P m^{-2}	[A7b]	

Appendix B: Soil-Plant Water Relations

Canopy Transpiration

$LE_{ci} = L (e_a - e_{ci(T_{ci}, \psi_{ci})}) / r_{ai}$	<i>LE</i> from canopy evaporation	[B1a]
$LE_{ci} = L (e_a - e_{ci(T_{ci}, \psi_{ci})}) / (r_{ai} + r_{ci}) - LE_{ci}$ from [B1a]	<i>LE</i> from canopy transpiration	[B1b]
$H_{ci} = \rho C_p (T_a - T_{ci}) / r_{ai}$	<i>H</i> from canopy energy balance	[B1c]
$r_{cmini} = 0.64 (C_b - C_i') / V_{c_i}'$	r_c driven by rates of carboxylation	[B2a]
$r_{ci} = r_{cmini} + (r_{cmaxi} - r_{cmini}) e^{(-\beta \psi_{ci})}$	vs. diffusion	[B2b]
$r_{ai} = \{(\ln((z_u - z_{di}) / z_{ri})^2 / (K^2 u_a))\} / (1 - 10 Ri)$	r_c constrained by water status	
$Ri = \{g (z_u - z_{ri}) / (u_a^2 T_a)\} (T_a - T_c)$	r_a driven by windspeed, surface	[B3a]
	r_a adjusted for stability vs. buoyancy	[B3b]
$\psi_{ci} = \psi_{ci} - \psi_{pi}$		[B4]

Root and Mycorrhizal Water Uptake

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

Canopy Water Potential

$$(e_a - e_{i(T_{ci})}) / (r_{ai} + r_{ci}) \text{ [B1]} = \sum_l \sum_r (\psi_{ci}' - \psi_s') / (\Omega_{si,r,l} + \Omega_{ti,r,l} + \sum_x \Omega_{ai,r,l,x}) + X_{ci} \delta \psi_{ci} / \delta t$$

[B14]
 ψ_c solved when transpiration from
 [B1-B4] (LHS) equals uptake from
 [B5-B13] + change in storage (RHS)

Definition of Variables in Appendix B

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	plant species or functional type: coniferous, deciduous, annual, perennial, C ₃ , C ₄ , monocot, dicot etc.				
<i>j</i>	branch or tiller				
<i>k</i>	node				
<i>l</i>	soil or canopy layer				
<i>m</i>	leaf azimuth				
<i>n</i>	leaf inclination				
<i>o</i>	leaf exposure (sunlit vs. shaded)				
<i>r</i>	root or mycorrhizae				
<i>variables</i>					
β	stomatal resistance shape parameter	MPa ⁻¹	[B2b,C4,C9]	-5.0	Grant and Flanagan (2007)
C_b	[CO ₂] in canopy air	μmol mol ⁻¹	[B2,C2,C5]		
$C_{i'}$	[CO ₂] in canopy leaves at $\psi_{ci} = 0$ MPa	μmol mol ⁻¹	[B2]	0.70 C_b	Larcher (2001)

$d_{i,r,l}$	half distance between adjacent roots	m	[B9]		
E_{ci}	canopy transpiration	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[B14]		
e_a	atmospheric vapor density at T_a and ambient humidity	g m^{-3}	[B1]		
$e_{ci(T_{ci}, \psi_{ci})}$	canopy vapor density at T_{ci} and ψ_{ci}	g m^{-3}	[B1]		
K	von Karman's constant		[B3a]	0.41	
$\kappa_{ri,r,l}$	hydraulic conductivity between soil and root surface	$\text{m}^2 \text{MPa}^{-1} \text{h}^{-1}$	[B9]		
γ	scaling factor for bole axial resistance from primary root axial resistance	-	[B11]	1.6×10^4	Grant et al. (2007)
L	latent heat of evaporation	J g^{-1}	[B1]	2460	
LE_i	latent heat flux between canopy and atmosphere	W m^{-2}	[B1]		
$L_{i,r,l}$	length of roots or mycorrhizae	m m^{-2}	[B9,B10,B12,B13]		
$M_{i,r,l}$	mass of roots or mycorrhizae	g m^{-2}	[B11,B13]		
$n_{i,r,l,x}$	number of primary ($x = 1$) or secondary ($x = 2$) axes	m^{-2}	[B11,B12]		
$\Omega_{ai,r}$	axial resistivity to water transport along root or mycorrhizal axes	MPa h m^{-4}	[B11,B12]	4.0×10^9 deciduous 1.0×10^{10} coniferous	Larcher (2001)
$\Omega_{ai,r,l,x}$	axial resistance to water transport along axes of primary ($x = 1$) or secondary ($x = 2$) roots or mycorrhizae	MPa h m^{-1}	[B6,B11,B12]		
$\Omega_{ri,r}$	radial resistivity to water transport from surface to axis of roots or mycorrhizae	MPa h m^{-2}	[B10]	1.0×10^4	Doussan et al. (1998)
$\Omega_{ri,r,l}$	radial resistance to water transport from surface to axis of roots or mycorrhizae	MPa h m^{-1}	[B6,B10]		
$\Omega_{si,r,l}$	radial resistance to water transport from soil to surface of roots or mycorrhizae	MPa h m^{-1}	[B6,B9]		
θ_{wl}	soil water content	$\text{m}^3 \text{m}^{-3}$	[B9]		

θ_{pl}	soil porosity	$\text{m}^3 \text{m}^{-3}$	[B9]		
$\theta_{p,i,r}$	root porosity	$\text{m}^3 \text{m}^{-3}$	[B13]		
Ri	Richardson number		[B3a,B3b]		van Bavel and Hillel (1976)
r_{ai}	aerodynamic resistance to vapor flux from canopy	s m^{-1}	[B1,B3a]		
r_{bi}	radius of bole at ambient ψ_{c_i}	m	[B11]		
r'_{b_i}	radius of bole at $\psi_{c_i} = 0$ MPa	m	[B11]		
r_{ci}	canopy stomatal resistance to vapor flux	s m^{-1}	[B1,B2b]		
r_{cmaxi}	canopy cuticular resistance to vapor flux	s m^{-1}	[B2b]	5.0×10^3	Larcher (2001)
r_{cmini}	minimum r_{c_i} at $\psi_{c_i} = 0$ MPa	s m^{-1}	[B2,B2b]		
$r_{i,r,l,x}$	radius of primary ($x=1$) or secondary ($x=2$) roots or mycorrhizae at ambient $\psi_{r_i,l,z}$	m	[B9,B11,B12,B13]		
$r'_{i,r}$	radius of secondary roots or mycorrhizae at $\psi_{r_i,l,z} = 0$ MPa	m	[B11,B12]	2.0×10^{-4} tree 1.0×10^{-4} bush 0.05×10^{-4} mycorrhizae	
ρ_r	root specific density	g C g FW^{-1}	[B13]	0.05	Grant (1998)
T_a	air temperature	K	[B3b]		
T_c	canopy temperature	K	[B3b]		
U_{wi}	total water uptake from all rooted soil layers	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[B5,B14]		
$U_{wi,r,l}$	water uptake by root and mycorrhizal surfaces in each soil layer	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[B5,B6]		
u_a	wind speed measured at z_u	m s^{-1}	[B3a,B3b]		
V'_{c_i}	potential canopy CO_2 fixation rate at $\psi_{c_i} = 0$ MPa	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[B2]		

v_r	root specific volume	$\text{m}^3 \text{g FW}^{-1}$	[B13]	10^{-6}	Grant (1998)
X_{ci}	canopy capacitance	$\text{m}^3 \text{m}^{-2} \text{MPa}^{-1}$	[B14]		
ψ_{ci}	canopy water potential	MPa	[B4,B7,B14]		
ψ'_{c_i}	$\psi_{ci} + \text{canopy gravitational potential}$	MPa	[B6,B7]		
$\psi_{\pi i}$	canopy osmotic potential	MPa	[B4]		
ψ_{sl}	soil water potential	MPa	[B8]		
ψ'_{s_l}	$\psi_{sl} + \text{soil gravitational potential}$	MPa	[B6,B8]		
ψ_{ti}	canopy turgor potential	MPa	[B2b,B4]	1.25 at $\psi_c = 0$	
z_{bi}	length of bole from soil surface to top of canopy	m	[B7,B11]		
z_{di}	canopy zero-plane displacement height	m	[B3a]		Perrier (1982)
z_l	depth of soil layer below surface	m	[B8,B11]		
z_r	canopy surface roughness	m	[B3a,B3b]		Perrier (1982)
z_u	height of wind speed measurement	m	[B3a,B3b]		

Appendix C: Gross Primary Productivity and Autotrophic Respiration

C₃ Gross Primary Productivity

$GPP = \sum_{i,j,k,l,m,n,o} (V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}) A_{i,j,k,l,m,n,o}$	solve for $C_{ii,j,k,l,m,n,o}$ at which	[C1]
$V_{gi,j,k,l,m,n,o} = (C_b - C_{ii,j,k,l,m,n,o})/r_{ii,j,k,l,m,n,o}$	diffusion	[C2]
$V_{ci,j,k,l,m,n,o} = \min\{V_{bi,j,k,l,m,n,o}, V_{ji,j,k,l,m,n,o}\}$	carboxylation	[C3]
$r_{ii,j,k,l,m,n,o} = r_{imini,j,k,l,m,n,o} + (r_{imaxi} - r_{imini,j,k,l,m,n,o}) e^{(-\beta\psi_i)}$	r_1 is leaf-level equivalent of r_c	[C4]
$r_{imini,j,k,l,m,n,o} = (C_b - C_i')/V_{ci,j,k,l,m,n,o}$	minimum r_1 is driven by carboxylation	[C5]
$V_{bi,j,k,l,m,n,o} = V_{bmaxi,j,k}(C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k})/(C_{ci,j,k,l,m,n,o} + K_{ci}) f_{\psi i,j,k,l,m,n,o} f_{NPi}$	CO ₂ , water, temperature and nutrient constraints on V_b	[C6a]
$V_{bmaxi,j,k} = V_{b'i} F_{rubisco_i} M_{i,j,k,prot}/A_{i,j,k} f_{tbi}$		[C6b]
$\Gamma_{i,j,k} = 0.5 O_c V_{omaxi,j,k} K_{ci} / (V_{bmaxi,j,k} K_{oi})$		[C6c]
$V_{omaxi,j,k} = V_{o'i} F_{rubisco_i} M_{i,j,k,prot}/A_{i,j,k} f_{toi}$		[C6d]
$K_{ci} = K_{ci} f_{tkci} (1 + O_c/K_{oi} f_{tkoi})$		[C6e]
$V_{ji,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o} Y_{i,j,k,l,m,n,o} f_{\psi i,j,k,l,m,n,o} f_{NPi}$		[C7]
$J_{i,j,k,l,m,n,o} = (\epsilon I_{i,l,m,n,o} + J_{maxi,j,k} - ((\epsilon I_{i,l,m,n,o} + J_{maxi,j,k})^2 - 4\alpha\epsilon I_{i,l,m,n,o} J_{maxi,j,k})^{0.5})/(2\alpha)$	water, temperature and nutrient constraints on V_j	[C8a]
$J_{maxi,j,k} = V_{j'i} F_{chlorophyll_i} M_{i,j,k,prot}/A_{i,j,k} f_{tji}$		[C8b]
$f_{\psi i,j,k,l,m,n,o} = (r_{imini,j,k,l,m,n,o} / r_{ii,j,k,l,m,n,o})^{0.5}$	non-stomatal effect related to stomatal effect	[C9]

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

Arrhenius functions for [C10a]

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

carboxylation, oxygenation and [C10b]

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

electron transport [C10c]

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

temperature sensitivity of \mathbf{K}_{c_i} , \mathbf{K}_{o_i} [C10d]

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

$$f_{NPI} = \min\{\sigma_{Ni,j}/(\sigma_{Ni,j} + \sigma_{Ci,j}/\mathbf{K}_{I\sigma_N}), \sigma_{Pi,j}/(\sigma_{Pi,j} + \sigma_{Ci,j}/\mathbf{K}_{I\sigma_P})\}$$

product inhibition of V_b , V_j [C11]

determined by σ_N and σ_P vs. σ_C in shoots

$$\delta M_{i,j,k,prot} / \delta t = \delta M_{i,j,k} / \delta t \min\{2.5 (N'_{leaf} + (N_{leaf} - N'_{leaf})), 25.0 (P'_{leaf} + (P_{leaf} - P'_{leaf}))\} f_{NPI}$$

leaf structural protein growth [C12]

Autotrophic Respiration

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

total autotrophic respiration [C13]

$$R_{ci,j} = \mathbf{R}_c' \sigma_{Ci,j} f_{tai}$$

O_2 constraint on root respiration [C14a]

$$R_{ci,r,l} = \mathbf{R}_c' \sigma_{Ci,r,l} f_{tai,l} (U_{O2i,r,l} / U'_{O2i,r,l})$$

from active uptake coupled with [C14b]

$$U_{O2i,r,l} = U'_{O2i,r,l} [O_{2ri,r,l}] / ([O_{2ri,r,l}] + \mathbf{K}_{O_2})$$

heterotrophic respiration in [A17], [C14c]

$$= U_{wi,r,l} [O_{2sl}] + 2\pi L_{i,r,l} D_{sO_2} ([O_{2sl}] - [O_{2ri,r,l}]) \ln\{(r_{sl} + r_{ri,r,l}) / r_{ri,r,l}\} + 2\pi L_{i,r,l} D_{rO_2} ([O_{2qi,r,l}] - [O_{2ri,r,l}]) \ln(r_{qi,r,l} / r_{ri,r,l})$$

and from active uptake coupled with diffusion of O_2 from roots [C14d]

$$U'_{O2i,r,l} = 2.67 R_{a'i,r,l}$$

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

remobilization when $R_m > R_c$ [C15]

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

maintenance respiration [C16]

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

growth when $R_m < R_c$ [C17]

Growth and Senescence

$$l_{i,j,z,C} = R_{si,j} C_{i,j,z=l,non-remobilizable} / C_{i,j,z=l,remobilizable} \quad \text{remobilization drives litterfall} \quad [C18]$$

$$l_{i,j,z,N,P} = l_{i,j,z,C} \mathbf{N}, \mathbf{P}_{\text{protein}} N_{i,j,z=l,non-remobilizable} / N_{i,j,z=l,remobilizable} \quad [C19]$$

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

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

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

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

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

$$f_{tai} = T_{ci} \{\exp[\mathbf{B}_v - \mathbf{H}_{av} / (RT_{ci})]\} / \{1 + \exp[(\mathbf{H}_{al} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - \mathbf{H}_{ah}) / (RT_{ci})]\} \quad \text{Arrhenius function for } R_a \quad [C22a]$$

$$f_{tmi} = e^{(0.0811 * (T_{ci} - 298.15))} \quad \text{temperature function for } R_m \quad [C22b]$$

Root and Mycorrhizal Nutrient Uptake

$$U_{NH4i,r,l} = \{U_{wi,r,l} [NH_4^+] + 2\pi L_{i,r,l} D_{eNH4l} ([NH_4^+] - [NH_4^+_{i,r,l}]) / \ln(d_{i,r,l} / r_{i,r,l})\} \quad \text{root N and P uptake from mass flow + diffusion coupled with active uptake of } NH_4^+, NO_3^- \text{ and } H_2PO_4^- \text{ constrained by } O_2 \text{ uptake, as for microbial N and P uptake [A26]} \quad [C23a]$$

$$= U'_{NH_4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NH_4^+_{i,r,l}] - [NH_4^+_{mn}]) / ([NH_4^+_{i,r,l}] - [NH_4^+_{mn}] + K_{NH_4}) f_{ij} f_{NPI} \quad [C23b]$$

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

$$= U'_{NO_3} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NO_3^-_{i,r,l}] - [NO_3^-_{mn}]) / ([NO_3^-_{i,r,l}] - [NO_3^-_{mn}] + K_{NO_3}) f_{ij} f_{NPI} \quad [C23d]$$

$$U_{PO4i,r,l} = \{U_{wi,r,l} [H_2PO_4^-] + 2\pi L_{i,r,l} D_{ePO4l} ([H_2PO_4^-] - [H_2PO_4^-_{i,r,l}]) / \ln(d_{i,r,l} / r_{i,r,l})\} \quad [C23e]$$

$$= U'_{PO_4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([H_2PO_4^-_{i,r,l}] - [H_2PO_4^-_{mn}]) / ([H_2PO_4^-_{i,r,l}] - [H_2PO_4^-_{mn}] + K_{PO_4}) f_{ij} f_{NPI} \quad [C23f]$$

$$f_{NPI} = \min\{\sigma_{Cij} / (\sigma_{Cij} + \sigma_{Ni,j} / K_{I\sigma_N}), \sigma_{Cij} / (\sigma_{Cij} + \sigma_{Pi,j} / K_{I\sigma_P})\} \quad \text{product inhibition of } U_{NH_4}, U_{NO_3} \text{ and } U_{PO_4} \text{ determined by } \sigma_N \text{ and } \sigma_P \text{ vs. } \sigma_C \text{ in roots} \quad [C23g]$$

C₄ Gross Primary Productivity

C₄ Mesophyll

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

$$V_{g(m4)ij,k,l,m,n,o} = (C_b - C_{i(m4)ij,k,l,m,n,o})/r_{fi,j,k,l,m,n,o}$$

gaseous diffusion [C25]

$$V_{c(m4)ij,k,l,m,n,o} = \min\{V_{b(m4)ij,k,l,m,n,o}, V_{j(m4)ij,k,l,m,n,o}\}$$

mesophyll carboxylation [C26]

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

[C27]

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

[C28]

$$V_{b(m4)ij,k,l,m,n,o} = V_{bmax(m4)ij,k}(C_{c(m4)ij,k,l,m,n,o} - \Gamma_{(m4)ij,k})/(C_{c(m4)ij,k,l,m,n,o} + K_{c(m4)ij,k})$$

CO₂-limited carboxylation [C29]

$$V_{j(m4)ij,k,l,m,n,o} = J_{(m4)ij,k,l,m,n,o} Y_{(m4)ij,k,l,m,n,o}$$

light-limited carboxylation [C30]

$$J_{(m4)ij,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{max(m4)ij,k} - ((\varepsilon I_{i,l,m,n,o} + J_{max(m4)ij,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{max(m4)ij,k})^{0.5})/(2\alpha)$$

irradiance response function [C31]

$$V_{bmax(m4)ij,k} = V_{bmax(m4)ij,k} [N_{pep(m4)ij,k}]' N_{fi,j,k} A_{fi,j,k} f_{C(m4)ij,k} f_{\psi i} f_{tvi}$$

PEPc activity [C32]

$$J_{max(m4)ij,k} = J_{max} [N_{chl(m4)ij,k}]' N_{fi,j,k} A_{fi,j,k} f_{C(m4)ij,k} f_{\psi i} f_{tvi}$$

chlorophyll activity [C33]

$$f_{C(m4)ij,k} = 1.0/(1.0 + [\chi_{C4(m4)ij,k}]/K_{\chi_{C4(m4)ij,k}})$$

C₄ product inhibition [C34]

$$f_{\psi ij,k,l,m,n,o} = (r_{fmini,j,k,l,m,n,o} / r_{fi,j,k,l,m,n,o})^{0.5}$$

non-stomatal water limitation [C35]

$$f_{tvi} = T_{ci} \{ \exp[B - H_a/(RT_{ci})] \} / \{ 1 + \exp[(H_{dl} - ST_{ci})/(RT_{ci})] + \exp[(ST_{ci} - H_{dh})/(RT_{ci})] \}$$

temperature limitation [C36]

C₄ Mesophyll-Bundle Sheath Exchange

$$V_{\chi_{C4(m4)ij,k}} = \kappa_{\chi_{C4(m4)}} (\chi_{C4(m4)ij,k} W_{lf(b4)ij,k} - \chi_{C4(b4)ij,k} W_{lf(m4)ij,k}) / (W_{lf(b4)ij,k} + W_{lf(m4)ij,k})$$

mesophyll-bundle sheath transfer [C37]

$$V_{\chi_{C4(b4)ij,k}} = \kappa_{\chi_{C4(b4)}} \chi_{C4(b4)ij,k} / (1.0 + C_{c(b4)ij,k} / K_{\chi_{C4(b4)}})$$

bundle sheath decarboxylation [C38]

$$V_{\phi(b4)ij,k} = \kappa_{C_c(b4)} (C_{c(b4)ij,k} - C_{c(m4)ij,k}) (12 \times 10^{-9}) W_{lf(b4)ij,k}$$

bundle sheath-mesophyll leakage [C39]

$$\delta \chi_{C4(m4)ij,k} / \delta t = \sum_{l,m,n,o} V_{c(m4)ij,k,l,m,n,o} - V_{\chi_{C4(m4)ij,k}}$$

mesophyll carboxylation products [C40]

$$\delta \chi_{C4(b4)ij,k} / \delta t = V_{\chi_{C4(m4)ij,k}} - V_{\chi_{C4(b4)ij,k}}$$

bundle sheath carboxylation products [C41]

$$\delta C_{c(b4)ij,k} / \delta t = V_{\chi C4(b4)ij,k} - V_{\phi(b4)ij,k} - \sum_{l,m,n,o} V_{c(b4)ij,k,l,m,n,o}$$

bundle sheath CO₂ concentration [C42]

C₄ Bundle Sheath

$$V_{c(b4)ij,k,l,m,n,o} = \min\{V_{b(b4)ij,k}, V_{j(b4)ij,k,l,m,n,o}\}$$

bundle sheath carboxylation [C43]

$$V_{b(b4)ij,k} = V_{\max(b4)ij,k} (C_{c(b4)ij,k} - \Gamma_{(b4)ij,k}) / (C_{c(b4)ij,k} + K_{c(b4)ij,k})$$

CO₂-limited carboxylation [C44]

$$V_{j(b4)ij,k,l,m,n,o} = J_{(b4)ij,k,l,m,n,o} Y_{(b4)ij,k}$$

light- limited carboxylation [C45]

$$J_{(b4)ij,k,l,m,n,o} = (\epsilon I_{i,l,m,n,o} + J_{\max(b4)ij,k} - ((\epsilon I_{i,l,m,n,o} + J_{\max(b4)ij,k})^2 - 4\alpha\epsilon I_{i,l,m,n,o} J_{\max(b4)ij,k})^{0.5}) / (2\alpha)$$

irradiance response function [C46]

$$V_{\max(b4)ij,k} = V_{\max(b4)ij,k}' [N_{\text{rub}(b4)ij,k}]' N_{\text{fi},j,k} A_{\text{fi},j,k} f_{C(c3)ij,k} f_{\psi i} f_{\text{vi}}$$

RuBPC activity [C47]

$$J_{\max(b4)ij,k} = J_{\max} [N_{\text{chl}(b4)ij,k}]' N_{\text{fi},j,k} A_{\text{fi},j,k} f_{C(c3)ij,k} f_{\psi i} f_{\text{vi}}$$

chlorophyll activity [C48]

$$f_{C(c3)ij,k} = \min\{[\nu_{\text{fi},j}] / ([\nu_{\text{fi},j}] + [\chi_{c3(b4)ij,k}] / K_{\text{I}\nu_{\text{P}}}), [\pi_{\text{fi},j}] / ([\pi_{\text{fi},j}] + [\chi_{c3(b4)ij,k}] / K_{\text{I}\pi_{\text{P}}})\}$$

C₃ product inhibition [C49]

Definition of Variables in Appendix C

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
<i>i</i>	species or functional type: evergreen, coniferous, deciduous, annual, perennial, C ₃ , C ₄ , 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>r</i>	root or mycorrhizae				
<i>z</i>	organ including leaf, root, mycorrhizae				

variables

A	leaf, root or mycorrhizal surface area	$\text{m}^2 \text{ m}^{-2}$	[C1,C6b,C6d,C8b,C21,C23,C32,C33,C47]		
β	shape parameter for stomatal effects on CO_2 diffusion and non-stomatal effects on carboxylation	MPa^{-1}	[C4 C27,C35,]	-5.0	Grant and Flanagan (2007)
B	parameter such that $f_t = 1.0$ at $T_c = 298.15 \text{ K}$		[C36]	17.533	
B_j	parameter such that $f_{ji} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10c]	17.363	
B_{kc}	parameter such that $f_{tkci} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10d]	22.187	
B_{ko}	parameter such that $f_{tkoi} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10e]	8.067	
B_o	parameter such that $f_{toi} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10b]	24.221	
B_v	parameter such that $f_{tvi} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10a, C22]	26.238	
C_b	$[\text{CO}_2]$ in canopy air	$\mu\text{mol mol}^{-1}$	[C2,C5 C25,C28]		
$C_{c(b4)}$	$[\text{CO}_2]$ in C_4 bundle sheath	μM	[C38,C39,C42,C44]		
$C_{c(m4)}$	$[\text{CO}_2]$ in C_4 mesophyll in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM	[C29,C39]		
C_c	$[\text{CO}_2]$ in canopy chloroplasts in equilibrium with $C_{ii,j,k,l,m,n,o}$	μM	[C6]		
$C_{i(m4)'}^1$	$[\text{CO}_2]$ in C_4 mesophyll air when $\psi_{ci} = 0$	$\mu\text{mol mol}^{-1}$	[C28]	$0.45 \times C_b$	
$C_{i(m4)}$	$[\text{CO}_2]$ in C_4 mesophyll air	$\mu\text{mol mol}^{-1}$	[C25]		
$C_{i,j,z=l}$	C content of leaf ($z = l$)	g C m^{-2}	[C18]		
C_i'	$[\text{CO}_2]$ in canopy leaves when $\psi_{ci} = 0$	$\mu\text{mol mol}^{-1}$	[C5]	$0.70 \times C_b$	Larcher (2001)

C_i	[CO ₂] in canopy leaves	$\mu\text{mol mol}^{-1}$	[C2]		
$D_{e \text{ NH}_4l}$	effective dispersivity-diffusivity of NH ₄ ⁺ during root uptake	$\text{m}^2 \text{h}^{-1}$	[C23]		
$D_{e \text{ NO}_3l}$	effective dispersivity-diffusivity of NO ₃ ⁻ during root uptake	$\text{m}^2 \text{h}^{-1}$	[C23]		
$D_{e \text{ PO}_4l}$	effective dispersivity-diffusivity of H ₂ PO ₄ ⁻ during root uptake	$\text{m}^2 \text{h}^{-1}$	[C23]		
D_{rO_2}	aqueous diffusivity of O ₂ from root aerenchyma to root or mycorrhizal surfaces	$\text{m}^2 \text{h}^{-1}$	[C14d]		
D_{sO_2}	aqueous diffusivity of O ₂ from soil to root or mycorrhizal surfaces	$\text{m}^2 \text{h}^{-1}$	[C14d]		
$d_{i,r,l}$	half distance between adjacent roots assumed equal to uptake path length	m	[C23]	$(\pi L_{s,z} / \Delta z)^{-1/2}$	Grant (1998)
$E_{N,P}$	energy cost of nutrient uptake	g C g N ⁻¹ or P ⁻¹	[C13]	2.15	Veen (1981)
$f_{C(c3)}$	C ₃ product inhibition of RuBP carboxylation activity in C ₄ bundle sheath or C ₃ mesophyll	–	[C47,C48,C49]		
$f_{C(m4)}$	C ₄ product inhibition of PEP carboxylation activity in C ₄ mesophyll	–	[C32,C33,C34]		
F_{chl}	fraction of leaf protein in chlorophyll	-	[C8b]	0.025	
f_{NPi}	N,P inhibition on carboxylation, leaf protein growth, root uptake	–	[C6a,C7,C11,C12,C23]		
$F_{rubisco}$	fraction of leaf protein in rubisco	-	[C6b,d]	0.125	
f_{tai}	temperature effect on $R_{ai,j}$	–	[C14, C22]		
f_{tbi}	temperature effect on carboxylation	–	[C6b,C10a]		
f_{tgl}	temperature function for root or mycorrhizal growth respiration	dimensionless	[C23]		
f_{tji}	temperature effect on electron transport		[C8b,C10c]		

f_{tkci}	temperature effect on K_{c_i}		[C6e,C10d]		Bernacchi et al. (2001,2003)
f_{tkoi}	temperature effect on K_{o_i}		[C6e,C10e]		Bernacchi et al. (2001,2003)
f_{tmi}	temperature effect on $R_{m_i,j}$	–	[C16, C22b]	$Q_{10} = 2.25$	
f_{toi}	temperature effect on oxygenation		[C6d,C10b]		
f_{tvi}	temperature effect on carboxylation	–	[C32,C33,C36,C4 7,C48]		
$f_{\psi i}$	non-stomatal water effect on carboxylation	–	[C6a,C7,C9]		Medrano et al. (2002)
$f_{\psi i}$	non-stomatal water effect on carboxylation	–	[C32,C33,C35C47 ,C48]		
H_a	energy of activation	$J\ mol^{-1}$	[C36]	57.5×10^3	
H_{aj}	energy of activation for electron transport	$J\ mol^{-1}$	[C10c]	43×10^3	Bernacchi et al. (2001,2003)
H_{akc}	parameter for temperature sensitivity of K_{c_i}	$J\ mol^{-1}$	[C10d]	55×10^3	Bernacchi et al. (2001,2003)
H_{ako}	parameter for temperature sensitivity of K_{o_i}	$J\ mol^{-1}$	[C10e]	20×10^3	Bernacchi et al. (2001,2003)
H_{ao}	energy of activation for oxygenation	$J\ mol^{-1}$	[C10b, C22]	60×10^3	Bernacchi et al. (2001,2003)
H_{av}	energy of activation for carboxylation	$J\ mol^{-1}$	[C10a, C22]	65×10^3	Bernacchi et al. (2001,2003)
H_{dh}	energy of high temperature deactivation	$J\ mol^{-1}$	[C10, C22]	222.5×10^3	
H_{dh}	energy of high temperature deactivation	$J\ mol^{-1}$	[C36]	220×10^3	
H_{dl}	energy of low temperature deactivation	$J\ mol^{-1}$	[C10, C22]	198.0×10^3	

H_{dl}	energy of low temperature deactivation	J mol^{-1}	[C36]	190×10^3	
I	irradiance	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C8a,]		
$J_{(b4)}$	electron transport rate in C_4 bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C45,C46]		
$J_{(m4)}$	electron transport rate in C_4 mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C30,C31]		
J	electron transport rate in C_3 mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C7,C8a]		
J_{\max}'	specific electron transport rate at non-limiting I and 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{s}^{-1}$	[C33,C48]	400	
$J_{\max(b4)}$	electron transport rate in C_4 bundle sheath at non-limiting I	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C46,C48]		
$J_{\max(m4)}$	electron transport rate in C_4 mesophyll at non-limiting I	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C31,C33]		
J_{\max}	electron transport rate at non-limiting I , ψ_{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_4 bundle sheath	μM	[C44]	30.0 at 25°C and zero O_2	Lawlor (1993)
$K_{c(m4)}$	Michaelis-Menten constant for carboxylation in C_4 mesophyll	μM	[C29]	3.0 at 25°C	Lawlor (1993)
K_c	Michaelis-Menten constant for carboxylation at zero O_2	μM	[C6c,C6e]	12.5 at 25°C	Farquhar et al. (1980)
K_c	Michaelis-Menten constant for carboxylation at ambient O_2	μM	[C6e]		
$K_{I/C4(b4)}$	constant for CO_2 product inhibition of C_4 decarboxylation in C_4 bundle sheath	μM	[C38]	1000.0	

$K_{I_{VC4(m4)}}$	constant for C ₄ product inhibition of PEP carboxylation activity in C ₄ mesophyll	μM	[C34]	5×10^6	
$K_{I_{Vf}}$	constant for C ₃ product inhibition of RuBP carboxylation activity in C ₄ bundle sheath or C ₃ mesophyll caused by [$V_{fi,j}$]	g C g N^{-1}	[C49]	100	
$K_{I_{\pi f}}$	constant for C ₃ product inhibition of RuBP carboxylation activity in C ₄ bundle sheath or C ₃ mesophyll caused by [$\pi_{fi,j}$]	g C g P^{-1}	[C49]	1000	
$K_{I_{\sigma N}}$	inhibition constant for $\sigma_{C_{i,j}}$ vs. σ_{N_j} in f_{NP} in shoots roots	g C g N^{-1} g N g C^{-1}	[C11] [C23]	100 (shoot) 0.1 (root)	Grant (1998)
$K_{I_{\sigma P}}$	inhibition constant for $\sigma_{C_{i,j}}$ vs. $\sigma_{P_{i,j}}$ in f_{NP} in shoots roots	g C g P^{-1} g P g C^{-1}	[C11] [C23]	1000 (shoot) 0.01 (root)	Grant (1998)
K_{NH_4}	M-M constant for NH ₄ ⁺ uptake at root or mycorrhizal surfaces	g N m^{-3}	[C23]	0.40	Barber and Silberbush, 1984
K_{NO_3}	M-M constant for NO ₃ ⁻ uptake at root or mycorrhizal surfaces	g N m^{-3}	[C23]	0.35	Barber and Silberbush, 1984
K_{PO_4}	M-M constant for H ₂ PO ₄ ⁻ uptake root or mycorrhizal surfaces	g P m^{-3}	[C23]	0.125	Barber and Silberbush, 1984
K_{O_2}	Michaelis-Menten constant for root or mycorrhizal O ₂ uptake	g m^{-3}	[C14c]	0.064	Griffin (1972)
K_{O_i}	inhibition constant for O ₂ in carboxylation	μM	[C6c,C6e]	500 at 25 °C	Farquhar et al. (1980)
L	root length	m m^{-2}	[C14d,C21b,C23]		
l_C	C litterfall from leaf or root	$\text{g C m}^{-2} \text{h}^{-1}$	[C18,C19,C20]		
$l_{N,P}$	N or P litterfall from leaf or root	$\text{g C m}^{-2} \text{h}^{-1}$	[C19]		
M_B	branch C phytomass	g C m^{-2}	[C20]		

M_L	leaf C phytomass	g C m^{-2}	[C12,C21]		
M_R	root C phytomass	g C m^{-2}	[C20,C21]		
M_{iprot}	leaf protein phytomass calculated from leaf N, P contents	g N m^{-2}	[C6b,C6d,C8b,C12]		
N,P	N or P content of organ z	g N m^{-2}	[C16, C19]		
N,P_{prot}	N or P content of protein remobilized from leaf or root	g N or P g C^{-1}	[C19]	0.4, 0.04	
$[\text{NH}_4^+_{i,r,l}]$	concentration of NH_4^+ at root or mycorrhizal surfaces	g N m^{-3}	[C23]		
$[\text{NH}_4^+_{mn}]$	concentration of NH_4^+ at root or mycorrhizal surfaces below which $U_{\text{NH}_4} = 0$	g N m^{-3}	[C23]	0.0125	Barber and Silberbush, 1984
$[\text{NO}_3^-_{i,r,l}]$	concentration of NO_3^- at root or mycorrhizal surfaces	g N m^{-3}	[C23]		
$[\text{NO}_3^-_{mn}]$	concentration of NO_3^- at root or mycorrhizal surfaces below which $U_{\text{NO}_3} = 0$	g N m^{-3}	[C23]	0.03	Barber and Silberbush, 1984
$[\text{H}_2\text{PO}_4^-_{i,r,l}]$	concentration of H_2PO_4^- root or mycorrhizal surfaces	g N m^{-3}	[C23]		
$[\text{H}_2\text{PO}_4^-_{mn}]$	concentration of H_2PO_4^- at root or mycorrhizal surfaces below which $U_{\text{PO}_4} = 0$	g N m^{-3}	[C23]	0.002	Barber and Silberbush, 1984
N_{leaf}	maximum leaf structural N content	g N g C^{-1}	[C12]	0.10	
N'_{leaf}	minimum leaf structural N content	g N g C^{-1}	[C12]	$0.33 \times N_{\text{leaf}}$	
N_{lf}	total leaf N	$\text{g N m}^{-2} \text{leaf}$	[C32,C33,C47,C48]		
$[N_{\text{chl}(b4)}]'$	ratio of chlorophyll N in C_4 bundle sheath to total leaf N	g N g N^{-1}	[C48]	0.05	
$[N_{\text{chl}(m4)}]'$	ratio of chlorophyll N in C_4 mesophyll to total leaf N	g N g N^{-1}	[C33]	0.05	
$[N_{\text{pep}(m4)}]'$	ratio of PEP carboxylase N in C_4 mesophyll to total leaf N	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	g N g N ⁻¹	[C47]	0.025
O _{2q}	aqueous O ₂ concentration in root or mycorrhizal aerenchyma	g m ⁻³	[C14c,d]	
O _{2r}	aqueous O ₂ concentration at root or mycorrhizal surfaces	g m ⁻³	[C14c,d]	
O _{2s}	aqueous O ₂ concentration in soil solution	g m ⁻³	[C14c,d]	
O _c	[O ₂] in canopy chloroplasts in equilibrium with O ₂ in atm.	μM	[C6c,C6e]	
P _{leaf}	maximum leaf structural P content	g P g C ⁻¹	[C12]	0.10
P' _{leaf}	minimum leaf structural P content	g P g C ⁻¹	[C12]	0.33 x P _{leaf}
[π_{if}]	concentration of nonstructural root P uptake product in leaf	g P g C ⁻¹	[C49]	
θ _P	root or mycorrhizal porosity	m ³ m ⁻³	[C21b]	0.1 – 0.5
R	gas constant	J mol ⁻¹ K ⁻¹	[C10, C22]	8.3143
<i>R</i>	gas constant	J mol ⁻¹ K ⁻¹	[C36]	8.3143
<i>R</i> _a	total autotrophic respiration	g C m ⁻² h ⁻¹	[C13]	
<i>R</i> _a '	<i>R</i> _a under nonlimiting O ₂	g C m ⁻² h ⁻¹	[C14]	
<i>R</i> _c '	specific autotrophic respiration of $\sigma_{\text{Ci},j}$ at $T_{\text{ci}} = 25$ °C	g C g C ⁻¹ h ⁻¹	[C14]	0.015
<i>R</i> _c	autotrophic respiration of $\sigma_{\text{Ci},j}$ or $\sigma_{\text{Ci},l}$	g C m ⁻² h ⁻¹	[C13,C14,C17, C15]	
<i>R</i> _g	growth respiration	g C m ⁻² h ⁻¹	[C17,C20]	
<i>r</i> _{i,r,l}	radius of root or mycorrhizae	m	[C23]	1.0 × 10 ⁻³ or 5.0 × 10 ⁻⁶
<i>r</i> _{if}	leaf stomatal resistance	s m ⁻¹	[C25,C27,C39]	

r_{lfmaxi}	leaf cuticular resistance	$s\ m^{-1}$	[C27]		
$r_{lfmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	$s\ m^{-1}$	[C27,C28,C35]		
$r_{li,j,k,l,m,n,o}$	leaf stomatal resistance	$s\ m^{-1}$	[C2,C4,C9]		
r_{lmaxi}	leaf cuticular resistance	$s\ m^{-1}$	[C4]		
$r_{lmini,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{ci} = 0$	$s\ m^{-1}$	[C4,C5,C9]		
R_m'	specific maintenance respiration of $\sigma_{Ci,j}$ at $T_{ci} = 25\ ^\circ C$	$g\ C\ g\ N^{-1}\ h^{-1}$	[C16]	0.0115	Barnes et al. (1998)
$R_{mi,j}$	above-ground maintenance respiration	$g\ C\ m^{-2}\ h^{-1}$	[C16,C17,C15]		
$r_{qi,r,l}$	radius of root aerenchyma	m	[C14d]		
$r_{ri,r,l}$	root radius	m	[C14d,C21b]		
$R_{si,j}$	respiration from remobilization of leaf C	$g\ C\ m^{-2}\ h^{-1}$	[C13,C15,C18, C20]		
r_{sl}	thickness of soil water films	m	[C14d]		
ρ_r	dry matter content of root biomass	$g\ g^{-1}$	[C21b]	0.125	
S	change in entropy	$J\ mol^{-1}\ K^{-1}$	[C10, C22]	710	Sharpe and DeMichelle (1977)
S	change in entropy	$J\ mol^{-1}\ K^{-1}$	[C36]	710	
σ_C	nonstructural C product of CO_2 fixation	$g\ C\ g\ C^{-1}$	[C11, C23]		
σ_N	nonstructural N product of root uptake	$g\ N\ g\ C^{-1}$	[C11, C23]		
σ_P	nonstructural P product of root uptake	$g\ P\ g\ C^{-1}$	[C11, C23]		

T_{ci}	canopy temperature	K	[C10, C22]		
T_{ci}	canopy temperature	°C	[C36]		
$U_{NH4i,r,l}$	NH_4^+ uptake by roots or mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$	[C23]		
U'_{NH4}	maximum U_{NH4} at 25 °C and non-limiting NH_4^+	$g\ N\ m^{-2}\ h^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{NO3i,r,l}$	NO_3^- uptake by roots or mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$	[C23]		
U'_{NO3}	maximum U_{NO3} at 25 °C and non-limiting NO_3^-	$g\ N\ m^{-2}\ h^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{PO4i,r,l}$	$H_2PO_4^-$ uptake by roots or mycorrhizae	$g\ N\ m^{-2}\ h^{-1}$	[C23]		
U'_{PO4}	maximum U_{PO4} at 25 °C and non-limiting $H_2PO_4^-$	$g\ N\ m^{-2}\ h^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{O2i,r,l}$	O_2 uptake by roots and mycorrhizae under ambient O_2	$g\ O\ m^{-2}\ h^{-1}$	[C14b,c,C23b,d,f]		
$U'_{O2i,l,r}$	O_2 uptake by roots and mycorrhizae under nonlimiting O_2	$g\ O\ m^{-2}\ h^{-1}$	[C14b,c,C23b,d,f]		
$U_{wi,r,l}$	root water uptake	$m^3\ m^{-2}\ h^{-1}$	[C14d,C23]		
$V_{\phi(b4)ij,k}$	CO_2 leakage from C_4 bundle sheath to C_4 mesophyll	$g\ C\ m^{-2}\ h^{-1}$	[C39,C42]		
V_b'	specific rubisco carboxylation at 25 °C	$\mu mol\ g^{-1}\ rubisco\ s^{-1}$	[C6b]	45	Farquhar et al. (1980)
$V_{b(b4)ij,k}$	CO_2 -limited carboxylation rate in C_4 bundle sheath	$\mu mol\ m^{-2}\ s^{-1}$	[C43,C44]		
$V_{b(m4)ijklmno}$	CO_2 -limited carboxylation rate in C_4 mesophyll	$\mu mol\ m^{-2}\ s^{-1}$	[C26]		
$V_{bij,klmno}$	CO_2 -limited leaf carboxylation rate	$\mu mol\ m^{-2}\ s^{-1}$	[C3,C6]		
$V_{bmax(b4)'}'$	RuBP carboxylase specific activity in C_4 bundle sheath at 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu mol\ g^{-1}\ s^{-1}$	[C47]	75	

$V_{\text{bmax}(b4)i,j,k}$	CO ₂ -nonlimited carboxylation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C44,C47]		
$V_{\text{bmax}(m4) '}$	PEP carboxylase specific activity in C ₄ mesophyll at 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{s}^{-1}$	[C32]	150	
$V_{\text{bmax}(m4)i,j,k}$	CO ₂ -nonlimited carboxylation rate in 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 CO ₂ , ψ_{ci} , T_c and N,P	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C6a,C6b,C6c]		
$V_{c(b4)i,j,k,l,m,n,o}$	CO ₂ fixation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C43]		
$V_{c(m4)i,j,k,l,m,n,o}$	CO ₂ fixation rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C24,C26,C40,C41]		
$V_{c0(m4) i,j,k,l,m,n,o}$	CO ₂ fixation rate in C ₄ mesophyll when $\psi_{ci} = 0$ MPa	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C28]		
$V_{ci,j,k,l,m,n,o}$	leaf CO ₂ fixation rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C1,C3]		
$V_c' i,j,k,l,m,n,o$	leaf CO ₂ fixation rate when $\psi_{ci} = 0$	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C5]		
$V_{g(m4)i,j,k,l,m,n,o}$	CO ₂ diffusion rate into C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C24,C25]		
$V_{gi,j,k,l,m,n,o}$	leaf CO ₂ diffusion rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C1,C2]		
V_j'	specific chlorophyll e ⁻ transfer at 25 °C	$\mu\text{mol g}^{-1} \text{chlorophyll s}^{-1}$	[C8b]	450	Farquhar et al. (1980)
$V_{j(b4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C43,C45]		
$V_{j(m4)i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C26,C30]		
$V_{ji,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C3,C7]		
V_o'	specific rubisco oxygenation at 25 °C	$\mu\text{mol g}^{-1} \text{rubisco s}^{-1}$	[C6d]	9.5	Farquhar et al. (1980)

$V_{\text{max}i,j,k}$	leaf oxygenation rate at non-limiting O_2 , ψ_{ci} , T_c and N,P	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C6c,d]	
$V_{\chi\text{C4}(b4)i,j,k}$	decarboxylation of C_4 fixation product in C_4 bundle sheath	$\text{g C m}^{-2} \text{h}^{-1}$	[C38,C41,C42]	
$V_{\chi\text{C4}(m4)}$	transfer of C_4 fixation product between C_4 mesophyll and bundle sheath	$\text{g C m}^{-2} \text{h}^{-1}$	[C37]	
$[V_{\text{lf}}]$	concentration of nonstructural root N uptake product in leaf	g N g C^{-1}	[C49]	
v_r	specific volume of root biomass	$\text{m}^3 \text{g}^{-1}$	[C21b]	
$W_{\text{lf}(b4)}$	C_4 bundle sheath water content	g m^{-2}	[C37,C39]	
$W_{\text{lf}(m4)}$	C_4 mesophyll water content	g m^{-2}	[C37]	
$Y_{(b4)}$	carboxylation yield from electron transport in C_4 bundle sheath	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C45]	
$Y_{(m4)}$	carboxylation yield from electron transport in C_4 mesophyll	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C30]	
Y_g	fraction of $\sigma_{C_{ij}}$ used for growth expended as $R_{g_{i,j,z}}$ by organ z	g C g C^{-1}	[C20]	0.28 ($z = \text{leaf}$), 0.24 ($z = \text{root and other non-foliar}$), 0.20 ($z = \text{wood}$)
y	plant population	m^{-2}	[C21]	
Y	carboxylation yield	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C7]	
Γ	CO_2 compensation point	μM	[C6a,C6c]	
$\Gamma_{(b4)}$	CO_2 compensation point in C_4 bundle sheath	μM	[C44]	

$\Gamma_{(m4)}$	CO ₂ compensation point in C ₄ mesophyll	μM	[C29]		
α	shape parameter for response of J to I	-	[C8a]	0.7	
α	shape parameter for response of J to I	-	[C31,C46]	0.75	
χ	area:mass ratio of leaf growth	m g ⁻³	[C21]	0.0125	Grant and Hesketh (1992)
$\chi_{C4(b4)}$	non-structural C ₄ fixation product in C ₄ bundle sheath	g C m ⁻²	[C37,C38,C41]		
$\chi_{C4(m4)}$	non-structural C ₄ fixation product in C ₄ mesophyll	g C m ⁻²	[C37,C40]		
$[\chi_{c3(b4)}]$	concentration of non-structural C ₃ fixation product in C ₄ bundle sheath	g g ⁻¹	[C49]		
$[\chi_{C4(m4)}]$	concentration of non-structural C ₄ fixation product in C ₄ mesophyll	μM	[C34]		
ε	quantum yield	μmol e ⁻ μmol quanta ⁻¹	[C8a]	0.45	Farquhar et al. (1980)
ε	quantum yield	μmol e ⁻ μmol quanta ⁻¹	[C31,C46]	0.45	Farquhar et al., (1980)
$\kappa_{Cc(b4)}$	conductance to CO ₂ leakage from C ₄ bundle sheath	h ⁻¹	[C39]	20	
ψ_t	canopy turgor potential	MPa	[C4]	1.25 at $\psi_c = 0$	

Appendix D: Soil Water, Heat, Gas and Solute Fluxes

Surface Water Flux

$Q_{rx(x,y)} = v_{x(x,y)} d_{mx,y} L_y(x,y)$	2D Manning equation in x (EW) and y (NS) directions	[D1]
$Q_{ry(x,y)} = v_{y(x,y)} d_{mx,y} L_x(x,y)$		
$d_{x,y} = \max(0, d_{w(x,y)} + d_{i(x,y)} - d_{s(x,y)}) d_{w(x,y)} / (d_{w(x,y)} + d_{i(x,y)})$	surface water depth	[D2]
$v_{x(x,y)} = R^{0.67} s_{x(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over E slope	[D3]
$v_{y(x,y)} = R^{0.67} s_{y(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over S slope	
$v_{x(x,y)} = -R^{0.67} s_{x(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over W slope	
$v_{y(x,y)} = -R^{0.67} s_{y(x,y)}^{0.5} / z_{r(x,y)}$	runoff velocity over N slope	
$\Delta(d_{w(x,y)} A_{x,y}) / \Delta t = Q_{r,x(x,y)} - Q_{r,x+1(x,y)} + Q_{r,y(x,y)} - Q_{r,y+1(x,y)} + P - E_{x,y} - Q_{wz(x,y,l)}$	2D kinematic wave theory for overland flow	[D4]
$R = s_r d_m / [2(s_r^2 + 1)0.5]$	wetted perimeter	[D5a]
$s_{x(x,y)} = 2abs[(Z + d_s + d_m)_{x,y} - (Z + d_s + d_m)_{x+1,y}] / (L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and pooled surface water in x (EW) and y (NS) directions	[D5b]
$s_{y(x,y)} = 2abs[(Z + d_s + d_m)_{x,y} - (Z + d_s + d_m)_{x,y+1}] / (L_{y(x,y)} + L_{y(x,y+1)})$		
$LE_l = L (e_a - e_{l(T_l, \psi_l)}) / r_{al}$	evaporation from surface litter	[D6a]
$LE_s = L (e_a - e_{s(T_s, \psi_s)}) / r_{as}$	evaporation from soil surface	[D6b]

Subsurface Water Flux

$Q_{wx(x,y,z)} = K'_x (\psi_{sx,y,z} - \psi_{sx+1,y,z})$	3D Richard's or Green-Ampt equation depending on saturation of source or target cell in x (EW), y (NS) and z (vertical) directions	[D7]
$Q_{wy(x,y,z)} = K'_y (\psi_{sx,y,z} - \psi_{sx,y+1,z})$		
$Q_{wz(x,y,z)} = K'_z (\psi_{sx,y,z} - \psi_{sx,y,z+1})$		

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

3D water transfer plus freeze-thaw [D8]

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

in direction x if source and destination cells are unsaturated [D9a]

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

in direction x if source cell is saturated [D9b]

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

in direction x if destination cell is saturated

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

in direction y if source and destination cells are unsaturated [D9a]

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

in direction y if source cell is saturated [D9b]

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

in direction y if destination cell is saturated

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

in direction z if source and destination cells are unsaturated [D9a]

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

in direction z if source cell is saturated [D9b]

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

in direction z if destination cell is saturated

Exchange with Water Table

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

if $\psi_{sx,y,z} > \psi' + 0.01(d_{zx,y,z} - d_t)$ for [D10]

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

all depths z from $d_{zx,y,z}$ to d_t
or if $d_{zx,y,z} > d_t$

Heat Flux

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

for each canopy, snow, residue and soil surface, depending on [D11]

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

exposure [D12]

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

3D conductive – convective heat flux among snowpack, surface

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

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

$$G_{x(x-1,y,z)} - G_{x(x,y,z)} + G_{y(x,y-1,z)} - G_{y(x,y,z)} + G_{z(x,y,z-1)} - G_{z(x,y,z)} + LQ_{f(x,y,z)} + c_{(x,y,z)} (T_{(x,y,z)} - T'_{(x,y,z)})/\Delta t = 0 \quad [D13]$$

3D general heat flux equation in snowpack, surface residue and soil layers

Gas Flux

$$Q_{dsyx,y,z} = a_{gsx,y,z} D_{d\gamma} (S'_{\gamma} f_{d,\gamma,y,z} [\gamma_{gs}]_{x,y,z} - [\gamma_{ss}]_{x,y,z}) \quad [D14a]$$

$$Q_{d\gamma x,y,z} = a_{grx,y,z} D_{d\gamma} (S'_{\gamma} f_{d,\gamma,y,z} [\gamma_{gr}]_{x,y,z} - [\gamma_{sr}]_{x,y,z}) \quad [D14b]$$

$$Q_{gsyzx,y,l} = g_{ax,y} \{ [\gamma_a] - \{2[\gamma_{gs}]_{x,y,l} D_{gsyz(x,y,l)}/L_{z(x,y,l)} + g_{ax,y} [\gamma_a]\} / \{2 D_{gsyz(x,y,l)}/L_{z(x,y,l)} + g_{ax,y}\} \} \quad [D15a]$$

$$Q_{dsyx,y,l} = a_{gsx,y,l} D_{d\gamma} (S'_{\gamma} f_{d,\gamma,x,y,l} [\gamma_a] - [\gamma_{ss}]_{x,y,l}) \quad [D15b]$$

$$Q_{gsyx(x,y,z)} = -Q_{wx(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gsyx(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x+1,y,z}) / (L_x(x,y,z) + L_x(x+1,y,z)) \quad [D16a]$$

$$Q_{gsyy(x,y,z)} = -Q_{wy(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gsyy(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y+1,z}) / (L_y(x,y,z) + L_y(x,y+1,z)) \quad [D16b]$$

$$Q_{gsyz(x,y,z)} = -Q_{wz(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gsyz(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x,y,z+1}) / (L_z(x,y,z) + L_z(x,y,z+1)) \quad [D16c]$$

$$Q_{g\gamma z(x,y,z)} = D_{g\gamma z(x,y,z)} ([\gamma_{gr}]_{x,y,z} - [\gamma_a]) / \sum_{1,z} L_z(x,y,z) \quad [D16d]$$

$$D_{gsyx(x,y,z)} = D'_{g\gamma} f_{g,x,y,z} [0.5(\theta_{gx,y,z} + \theta_{gx+1,y,z})]^2 / \theta_{psx,y,z}^{0.67} \quad [D17a]$$

$$D_{gsyy(x,y,z)} = D'_{g\gamma} f_{g,x,y,z} [0.5(\theta_{gx,y,z} + \theta_{gx,y+1,z})]^2 / \theta_{psx,y,z}^{0.67} \quad [D17b]$$

$$D_{gsyz(x,y,z)} = D'_{g\gamma} f_{g,x,y,z} [0.5(\theta_{gx,y,z} + \theta_{gx,y,z+1})]^2 / \theta_{psx,y,z}^{0.67} \quad [D17c]$$

$$D_{g\gamma z(x,y,z)} = D'_{g\gamma} f_{g,x,y,z} \theta_{pfx,y,z}^{1.33} A_r(x,y,z) / A_{x,y} \quad [D17d]$$

$$Q_{b\gamma z} = \min[0.0, \{ (44.64 \theta_{wx,y,z} 273.16/T_{(x,y,z)} - \sum_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,\gamma,y,z} M_{\gamma})) \}] \quad [D18]$$

$$([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,\gamma,y,z} M_{\gamma})) / \sum_{\gamma} ([\gamma_s]_{x,y,z} / (S'_{\gamma} f_{d,\gamma,y,z} M_{\gamma})) S'_{\gamma} f_{d,\gamma,y,z} M_{\gamma} V_{x,y,z}$$

volatilization – dissolution

between aqueous and gaseous

phases in soil and root

volatilization – dissolution

between gaseous and aqueous

phases at the soil surface ($z = l$)

and the atmosphere

3D convective - conductive gas

flux among soil layers in x (EW), y

(NS) and z (vertical) directions,

convective - conductive gas

flux between roots and the

atmosphere

gaseous diffusivity as a function

of air-filled porosity in soil

gaseous diffusivity as a function

of air-filled porosity in roots

bubbling (-ve flux) when total of

all partial gas pressures exceeds

atmospheric pressure

Solute Flux

$Q_{syx}(x,y,z) = -Q_{wx}(x,y,z) [\gamma_s]_{x,y,z} + 2 D_{syx}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x+1,y,z}) / (L_x(x,y,z) + L_x(x+1,y,z))$	3D convective - dispersive solute flux among soil layers in x (EW), y (NS) and z (vertical) directions	[D19]
$Q_{syy}(x,y,z) = -Q_{wy}(x,y,z) [\gamma_s]_{x,y,z} + 2 D_{syy}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y+1,z}) / (L_y(x,y,z) + L_y(x,y+1,z))$		
$Q_{syz}(x,y,z) = -Q_{wz}(x,y,z) [\gamma_s]_{x,y,z} + 2 D_{syz}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y,z+1}) / (L_z(x,y,z) + L_z(x,y,z+1))$		
$D_{syx}(x,y,z) = D_{qx}(x,y,z) Q_{wx}(x,y,z) + D'_{sy} f_{sx,y,z} [0.5(\theta_{wx,y,z} + \theta_{wx+1,y,z})] \tau$	aqueous dispersivity as functions of water flux and water-filled porosity	[D20]
$D_{syy}(x,y,z) = D_{qy}(x,y,z) Q_{wy}(x,y,z) + D'_{sy} f_{sx,y,z} [0.5(\theta_{wx,y,z} + \theta_{wx+1,y,z})] \tau$		
$D_{syz}(x,y,z) = D_{qz}(x,y,z) Q_{wz}(x,y,z) + D'_{sy} f_{sx,y,z} [0.5(\theta_{wx,y,z} + \theta_{wx+1,y,z})] \tau$		
$D_{qx}(x,y,z) = 0.5 \alpha (L_x(x,y,z) + L_x(x+1,y,z))^\beta$	dispersivity as a function of water flow length	[D21]
$D_{qy}(x,y,z) = 0.5 \alpha (L_y(x,y,z) + L_y(x,y+1,z))^\beta$		
$D_{qz}(x,y,z) = 0.5 \alpha (L_z(x,y,z) + L_z(x,y,z+1))^\beta$		

Definition of Variables in Appendix D

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
x	grid cell position in west to east direction				
y	grid cell position in north to south direction				
z	grid cell position in vertical direction			$z = 0$: surface residue, $z = 1$ to n : soil layers	
<i>variables</i>					
A	area of landscape position	m^2	[D17c]		
A_r	root cross-sectional area of landscape position	m^2	[D17c]		
a_{gr}	air-water interfacial area in roots	$m^2 m^{-2}$	[D14b]		

a_{gs}	air-water interfacial area in soil	$m^2 m^{-2}$	[D14a,D15b]		Skopp (1985)
α	dependence of D_q on L	-	[D21]		
β	dependence of D_q on L	-	[D21]		
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 γ	$m^2 h^{-1}$	[D14,D15a]		
$D_{gr\gamma}$	gaseous diffusivity of gas γ in roots	$m^2 h^{-1}$	[D16d,D17d]		Luxmoore et al. (1970a,b)
$D_{gs\gamma}$	gaseous diffusivity of gas γ in soil	$m^2 h^{-1}$	[D15a,D16a,b,c,D17a,b,c]		Millington and Quirk (1960)
$D'_{g\gamma}$	diffusivity of gas γ in air at 0 °C	$m^2 h^{-1}$	[D17]	6.43×10^{-2} for $\gamma = O_2$	Campbell (1985)
D_q	dispersivity	m	[D20,D21]		
$D_{s\gamma}$	aqueous diffusivity of gas or solute γ	$m^2 h^{-1}$	[D19,D20]		
$D'_{s\gamma}$	diffusivity of gas γ in water at 0 °C	$m^2 h^{-1}$	[D20]	8.57×10^{-6} for $\gamma = O_2$	Campbell (1985)
d_m	depth of mobile surface water	m	[D1,D2,D5a,D6]		
d_i	depth of surface ice	m	[D2]		
d_s	maximum depth of surface water storage	m	[D2,D5b]		
d_t	depth of external water table	m	[D10]		
d_w	depth of surface water	m	[D1,D2]		
d_z	depth to mid-point of soil layer	m	[D10]		
E	evaporation or transpiration flux	$m^3 m^{-2} h^{-1}$	[D4,D11]		

e_a	atmospheric vapor density	$\text{m}^3 \text{m}^{-3}$	[D6]	
$e_{l(T_l, \psi_l)}$	surface litter vapor density at current T_l and ψ_l	g m^{-3}	[D6a]	
$e_{s(T_s, \psi_s)}$	soil surface vapor density at current T_s and ψ_s	g m^{-3}	[D6b]	
f_{d_γ}	temperature dependence of S'_γ	-	[D14,D15b,D18]	Wilhelm et al. (1977)
f_{g_γ}	temperature dependence of $D'_{g\gamma}$	-	[D17]	Campbell (1985)
f_{s_γ}	temperature dependence of $D'_{s\gamma}$	-	[D20]	Campbell (1985)
G	soil surface heat flux	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D11]	
G_x, G_y, G_z	soil heat flux in x, y or z directions	$\text{MJ m}^{-2} \text{h}^{-1}$	[D12,D13]	
g_a	boundary layer conductance	m h^{-1}	[D15a]	
γ	gas ($\text{H}_2\text{O}, \text{CO}_2, \text{O}_2, \text{CH}_4, \text{NH}_3, \text{N}_2\text{O}, \text{N}_2, \text{H}_2$) or solute (from appendix E)		[D14,D15]	
$[\gamma_a]$	atmospheric concentration of gas γ	g m^{-3}	[D15,D16d]	
$[\gamma_{gr}]$	gaseous concentration of gas γ in roots	g m^{-3}	[D14b,D16d]	
$[\gamma_{gs}]$	gaseous concentration of gas γ in soil	g m^{-3}	[D14a,D15a,D16a, D16b,D16c]	
$[\gamma_{sr}]$	aqueous concentration of gas γ in roots	g m^{-3}	[D14b]	
$[\gamma_{ss}]$	aqueous concentration of gas γ in soil	g m^{-3}	[D14a,D15b,D18, D19]	
H	sensible heat flux	$\text{MJ m}^{-2} \text{h}^{-1}$	[D11]	
K	hydraulic conductivity	$\text{m}^2 \text{MPa}^{-1} \text{h}^{-1}$	[D9,D10]	Green and Corey (1971)
K'_x, K'_y, K'_z	hydraulic conductance in x, y or z directions	$\text{m MPa}^{-1} \text{h}^{-1}$	[D7,D9]	
κ	thermal conductivity	$\text{MJ m}^{-1} \text{h}^{-1} \text{°C}^{-1}$	[D12]	de Vries (1963)

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	[D1,D5b,D8,D9,D10,D12,D15a,D16,D19]	
LE_1	latent heat flux from surface litter	[D6a]	$\text{MJ m}^{-2} \text{h}^{-1}$	
LE_s	latent heat flux from soil surface	[D6b]	$\text{MJ m}^{-2} \text{h}^{-1}$	
L	latent heat of evaporation	MJ m^{-3}	[D6,D11,D13]	2460
M_γ	atomic mass of gas γ	g mol^{-1}	[D18]	
P	precipitation flux	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D4]	
Q_{byz}	bubbling flux	$\text{g m}^{-2} \text{h}^{-1}$	[D18]	
Q_{dry}	volatilization – dissolution of gas γ between aqueous and gaseous phases in roots	$\text{g m}^{-2} \text{h}^{-1}$	[D14b]	
$Q_{\text{ds}\gamma}$	volatilization – dissolution of gas γ between aqueous and gaseous phases in soil	$\text{g m}^{-2} \text{h}^{-1}$	[D14a,D15b]	
Q_f	freeze-thaw flux (thaw +ve)	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D8,D13]	
$Q_{\text{gr}\gamma}$	gaseous flux of gas γ between roots and the atmosphere	$\text{g m}^{-2} \text{h}^{-1}$	[D16d]	
$Q_{\text{gs}\gamma}$	gaseous flux of gas γ in soil	$\text{g m}^{-2} \text{h}^{-1}$	[D15a,D16a,b,c]	
$Q_{\text{rx}}, Q_{\text{ry}}$	surface water flow in x or y directions	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D1,D4]	
Q_{sy}	aqueous flux of gas or solute γ	$\text{g m}^{-2} \text{h}^{-1}$	[D19]	
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]	
$Q_{\text{wx}}, Q_{\text{wy}}, Q_{\text{wz}}$	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]	
θ_g	air-filled porosity	$\text{m}^3 \text{m}^{-3}$	[D17a,b,c]	

θ_{pr}	root porosity	$m^3 m^{-3}$	[D17d]	dryland spp. 0.10 wetland spp. 0.20	Luxmoore et al. (1970a,b)
θ_{ps}	soil porosity	$m^3 m^{-3}$	[D17a,b,c]		
θ_w	water-filled porosity	$m^3 m^{-3}$	[D8,D18,D20]		
R	ratio of cross-sectional area to perimeter of surface flow	m	[D3,D5a]		
R_n	net radiation	$MJ m^{-2} h^{-1}$	[D11]		
r_{al}	surface litter boundary layer resistance	$m h^{-1}$	[D6a]		
r_{as}	Soil surface boundary layer resistance	$m h^{-1}$	[D6b]		
S'_γ	Ostwald solubility coefficient of gas γ at 30 °C	-	[D14,D15b,D18]	0.0293 for $\gamma = O_2$	Wilhelm et al. (1977)
s_r	slope of channel sides during surface flow	$m m^{-1}$	[D5a]		
s_x, s_y	slope in x or y directions	$m m^{-1}$	[D3,D5b]		
T	soil temperature	°C	[D12,D18]		
τ	tortuosity	-	[D20]		
v_x, v_y	velocity of surface flow in x or y directions	$m h^{-1}$	[D1,D3]		
ψ'	soil water potential at saturation	MPa	[D10]	5.0×10^{-3}	
ψ_s	soil water potential	MPa	[D7,D10]		
Z	surface elevation	m	[D5b]		
z_r	Manning's roughness coefficient	$m^{-1/3} h$	[D3]	0.01	

Appendix E: Solute Transformations

Precipitation - Dissolution Equilibria

$\text{Al}(\text{OH})_{3(s)} \Leftrightarrow (\text{Al}_{3+}^{3+}) + 3 (\text{OH}^-)$	(amorphous $\text{Al}(\text{OH})_3$)	-33.0	[E.1] ¹
$\text{Fe}(\text{OH})_{3(s)} \Leftrightarrow (\text{Fe}_{2+}^{2+}) + 3 (\text{OH}^-)$	(soil Fe)	-39.3	[E.2]
$\text{CaCO}_{3(s)} \Leftrightarrow (\text{Ca}_{2+}^{2+}) + (\text{CO}_3^{2-})$	(calcite)	-9.28	[E.3]
$\text{CaSO}_{4(s)} \Leftrightarrow (\text{Ca}_{2+}^{2+}) + (\text{SO}_4^{2-})$	(gypsum)	-4.64	[E.4] ²
$\text{AlPO}_{4(s)} \Leftrightarrow (\text{Al}_{3+}^{3+}) + (\text{PO}_4^{3-})$	(variscite)	-22.1	[E.5] ²
$\text{FePO}_{4(s)} \Leftrightarrow (\text{Fe}^{2+}) + (\text{PO}_4^{3-})$	(strengite)	-26.4	[E.6]
$\text{Ca}(\text{H}_2\text{PO}_4)_{2(s)} \Leftrightarrow (\text{Ca}^{2+}) + 2 (\text{H}_2\text{PO}_4^-)$	(monocalcium phosphate)	-1.15	[E.7] ³
$\text{CaHPO}_{4(s)} \Leftrightarrow (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	(monetite)	-6.92	[E.8]
$\text{Ca}_5(\text{PO}_4)_3\text{OH}_{(s)} \Leftrightarrow 5 (\text{Ca}^{2+}) + 3 (\text{PO}_4^{3-}) + (\text{OH}^-)$	(hydroxyapatite)	-58.2	[E.9]

*Cation Exchange Equilibria*⁴

$\text{X-Ca} + 2 (\text{NH}_4^+) \Leftrightarrow 2 \text{X-NH}_4 + (\text{Ca}^{2+})$		1.00	[E.10]
$3 \text{X-Ca} + 2 (\text{Al}^{3+}) \Leftrightarrow 2 \text{X-Al} + 3 (\text{Ca}^{2+})$		1.00	[E.11]
$\text{X-Ca} + (\text{Mg}^{2+}) \Leftrightarrow \text{X-Mg} + (\text{Ca}^{2+})$		0.60	[E.12]
$\text{X-Ca} + 2 (\text{Na}^+) \Leftrightarrow 2 \text{X-Na} + (\text{Ca}^{2+})$		0.16	[E.13]
$\text{X-Ca} + 2 (\text{K}^+) \Leftrightarrow 2 \text{X-K} + (\text{Ca}^{2+})$		3.00	[E.14]
$\text{X-Ca} + 2 (\text{H}^+) \Leftrightarrow 2 \text{X-H} + (\text{Ca}^{2+})$		1.00	[E.15]

Anion Adsorption Equilibria

$\text{X-OH}_2^+ \Leftrightarrow \text{X-OH} + (\text{H}^+)$		-7.35	[E.16]
$\text{X-OH} \Leftrightarrow \text{X-O}^- + (\text{H}^+)$		-8.95	[E.17]
$\text{X-H}_2\text{PO}_4 + \text{H}_2\text{O} \Leftrightarrow \text{X-OH}_2^+ + (\text{H}_2\text{PO}_4^-)$		-2.80	[E.18]
$\text{X-H}_2\text{PO}_4 + (\text{OH}^-) \Leftrightarrow \text{X-OH} + (\text{H}_2\text{PO}_4^-)$		4.20	[E.19]
$\text{X-HPO}_4 + (\text{OH}^-) \Leftrightarrow \text{X-OH} + (\text{HPO}_4^{2-})$		2.60	[E.20]

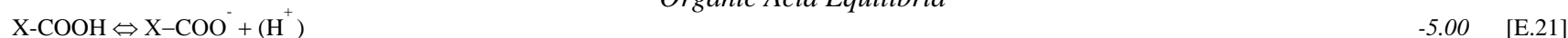
¹ Round brackets denote solute activity. Numbers in italics denote log *K* (precipitation-dissolution, ion pairs), Gapon coefficient (cation exchange) or log *c* (anion exchange).

² 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.

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

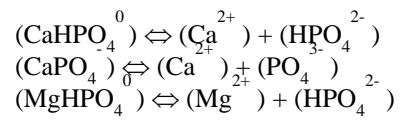
⁴ X- denotes surface exchange site for cation or anion adsorption.

Organic Acid Equilibria



Ion Pair Equilibria





-2.74 [E.53]

-6.46 [E.54]

-2.91 [E.55]

Appendix F: Symbiotic N₂ Fixation

Microbial Growth

$R_{\max,i,l} = M_{ni,l} R' [\chi_{ni,l}] / ([\chi_{ni,l}] + K_{\chi n}) f_t f_{NP}$	respiration demand	[F1]
$f_t = T_l \{ \exp[B - H_a/(RT_l)] \} / \{ 1 + \exp[(H_{dl} - ST_l)/(RT_l)] + \exp[(ST_l - H_{dh})/(RT_l)] \}$	Arrhenius function	[F2]
$f_{NP} = \min\{ [N_{ni,l}] / [N_n'], [P_{ni,l}] / [P_n'] \}$	N or P limitation	[F3]
$R_{i,l} = R_{\max,i,l} (V_{O_2i,l} / V_{O_2\max,i,l})$	O ₂ limitation	[F4]
$V_{O_2\max,i,l} = 2.67 R_{\max,i,l}$	O ₂ demand	[F5]
$V_{O_2i,l} = V_{O_2\max,i,l} [O_{2ri,l}] / ([O_{2ri,l}] + K_{O_2r})$	equilibrate O ₂ uptake with	[F6a]
$= 2\pi L_{ri,l} D_{sO_2} ([O_2] - [O_{2ri,l}]) / \ln((r_{ri,l} + r_{wl}) / r_{ri,l})$	supply	[F6b]
$R_{mi,l} = R_m N_{ni,l} f_{tm}$	maintenance respiration	[F7]
$f_{tm} = e^{[y(T_l - 298.16)]}$	temperature function	[F8]
$R_{gi,l} = \max\{0.0, R_{i,l} - R_{mi,l}\}$	growth + fixation respiration	[F9]
$R_{si,l} = \max\{0.0, R_{mi,l} - R_{i,l}\}$	microbial senescence	[F10]
$L_{Ci,l} = R_{si,l} \min\{ M_{ni,l} / (2.5N_{ni,l}), M_{ni,l} / (25.0P_{ni,l}) \}$	microbial C litterfall	[F11]

N₂ Fixation

$V_{N_2i,l} = \min\{ R_{gi,l} E_{N_2}' f_{CP}, M_{ni,l} [N_n'] - N_{ni,l} \} [N_{2ri,l}] / ([N_{2ri,l}] + K_{N_2r})$	rate of N ₂ fixation	[F12]
$f_{CP} = \min\{ [\chi_{ni,l}] / (1.0 + [v_{ni,l}] / K_{I\chi_n}), [\tau_{ni,l}] / (1.0 + [v_{ni,l}] / K_{I\tau_n}) \}$	product inhibition of N ₂ fixation	[F13]

$$R_{N2i,l} = V_{N2i,l} / E_{N2}'$$

$$U_{\chi i,l} = (R_{gi,l} - R_{N2i,l}) / (1 - Y_n')$$

$$\delta M_{ni,l} / \delta t = U_{i,l} Y_n' - L_{Ci,l}$$

$$\delta N_{ni,l} / \delta t = \delta M_{ni,l} / \delta t \min\{v_{ni,l} / \chi_{ni,l}, [N_n']\}$$

$$\delta N_{ni,l} / \delta t = N_{ni,l} / M_{ni,l} \delta M_{ni,l} / \delta t$$

$$\delta P_{ni,l} / \delta t = \delta M_{ni,l} / \delta t \min\{\pi_{ni,l} / \chi_{ni,l}, [P_n']\}$$

$$\delta P_{ni,l} / \delta t = P_{ni,l} / M_{ni,l} \delta M_{ni,l} / \delta t$$

$$L_{Ni,l} = \text{abs}(\delta N_{ni,l} / \delta t)$$

$$L_{Pi,l} = \text{abs}(\delta P_{ni,l} / \delta t)$$

fixation respiration

[F14]

growth respiration

[F15]

microbial C growth

[F16]

microbial N growth

$$\delta M_{ndi,l} / \delta t > 0$$

[F17a]

microbial N growth

$$\delta M_{ndi,l} / \delta t < 0$$

[F17b]

microbial P growth

$$\delta M_{ndi,l} / \delta t > 0$$

[F18a]

microbial P growth

$$\delta M_{ndi,l} / \delta t < 0$$

[F18b]

microbial N litterfall

$$\delta N_{ndi,l} / \delta t < 0$$

[F19]

microbial P litterfall

$$\delta P_{ndi,l} / \delta t < 0$$

[F20]

Nodule – Root Exchange

$$V_{\chi i,l} = \kappa (\chi_{vi,l} M_{ni,l} - \chi_{ni,l} M_{vi,l}) / (M_{ni,l} + M_{vi,l})$$

$$V_{vi,l} = \kappa (v_{vi,l} \chi_{ni,l} - v_{ni,l} \chi_{vi,l}) / (\chi_{ni,l} + \chi_{vi,l})$$

$$V_{\pi i,l} = \kappa (\pi_{vi,l} \chi_{ni,l} - \pi_{ni,l} \chi_{vi,l}) / (\chi_{ni,l} + \chi_{vi,l})$$

$$\delta \chi_{ni,l} / \delta t = V_{\chi i,l} - \min\{R_{mi,l}, R_{i,l}\} - R_{N2i,l} - U_{\chi i,l} + F_{LC,l} L_{Ci,l}$$

$$\delta v_{ni,l} / \delta t = V_{vi,l} - \delta N_{ni,l} / \delta t + V_{N2i,l} + F_{LN,l} L_{Ni,l}$$

$$\delta \pi_{ni,l} / \delta t = V_{\pi i,l} - \delta P_{ni,l} / \delta t + F_{LP,l} L_{Pi,l}$$

nodule–root C exchange

[F21]

nodule–root N exchange

[F22]

nodule–root P exchange

[F23]

nodule nonstructural C

[F24]

nodule nonstructural N

[F25]

nodule nonstructural P

[F26]

Definition of Variables in Appendix F

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

H_{dh}	energy of high temperature deactivation	J mol^{-1}	F2	220×10^3
H_{dl}	energy of low temperature deactivation	J mol^{-1}	F2	190×10^3
K_{zn}	Michaelis-Menten constant for nodule respiration of $\chi_{ndi,l}$	g g^{-1}	F1	0.01
K_{Izn}	inhibition constant for nonstructural N:C on N_2 fixation	g g^{-1}	F13	10
K_{Ipn}	inhibition constant for nonstructural N:P on N_2 fixation	g g^{-1}	F13	1000
K_{N_2r}	Michaelis-Menten constant for nodule N_2 uptake	g N m^{-3}	F12	0.14
K_{O_2r}	Michaelis-Menten constant for nodule O_2 uptake	g O m^{-3}	F6a	
κ	rate constant for nonstructural C,N,P exchange between root and nodule	h^{-1}	F21,F22,F23	
$L_{vi,l}$	root length	m m^{-2}	F6b	
$L_{Ci,l}$	nodule C litterfall	$\text{g C m}^{-2} \text{h}^{-1}$	F11,F16,F24	
$L_{Ni,l}$	nodule N litterfall	$\text{g N m}^{-2} \text{h}^{-1}$	F19,F25	
$L_{Pi,l}$	nodule P litterfall	$\text{g P m}^{-2} \text{h}^{-1}$	F20,F26	
$M_{ni,l}$	nodule structural C	g C m^{-2}	F1,F11,F12,F16 ,F17,F18,F21	
$M_{vi,l}$	root structural C	g C m^{-2}	F21	
$[N_n']$	maximum nodule structural N concentration	g N g C^{-1}	F3,F12	0.1

$N_{ni,l}$	nodule structural N	g N m^{-2}	F7,F11,F12,F17,F19,F25	
$[N_{ni,l}]$	nodule structural N concentration	g N g C^{-1}	F3,F17a	
$[N_{2ri,l}]$	rhizosphere aqueous N_2 concentration	g N m^{-3}	F12	
$v_{ni,l}$	nodule nonstructural N	g N m^{-2}	F17a,F22,F25	
$v_{ri,l}$	root nonstructural N	g N m^{-2}	F22	
$[v_{ni,l}]$	nodule concentration of nonstructural N	g g^{-1}	F13,F17a	
$[O_{2ri,l}]$	rhizosphere aqueous O_2 concentration	g O m^{-3}	F6a,b	
$[O_{2l}]$	soil aqueous O_2 concentration	g O m^{-3}	F6b	
$[P_n']$	maximum nodule structural P concentration	g P g C^{-1}	F3,F18a	0.01
$P_{ni,l}$	nodule structural P	g P m^{-2}	F18a,F20,F26	
$[P_{ni,l}]$	nodule structural P concentration	g P g C^{-1}	F3,F11	
$\pi_{ni,l}$	nodule nonstructural P	g P m^{-2}	F18a,F23,F26	
$\pi_{ri,l}$	root nonstructural P	g P m^{-2}	F23	
$[\pi_{ni,l}]$	nodule concentration of nonstructural P	g g^{-1}	F13	
R	gas constant	$\text{J mol}^{-1} \text{K}^{-1}$	F2	8.3143
$R_{gi,l}$	nodule growth respiration	$\text{g C m}^{-2} \text{h}^{-1}$	F9,F12,F15	

R'	specific nodule respiration at 25°C, and non-limiting O ₂ , $\chi_{ndi,l}$, $V_{ndi,l}$ and $\pi_{ndi,l}$	h ⁻¹	F1	0.125
$R_{i,l}$	nodule respiration under ambient O ₂	g C m ⁻² h ⁻¹	F4,F9,F10,F24	
R_m	specific nodule maintenance respiration at 25°C	g C g C ⁻¹ h ⁻¹	F7	
$R_{maxi,l}$	nodule respiration under non-limiting O ₂	g C m ⁻² h ⁻¹	F1,F4,F5	
$R_{mi,l}$	nodule maintenance respiration	g C m ⁻² h ⁻¹	F7,F9,F10,F24	
$R_{N_2i,l}$	nodule respiration for N ₂ fixation	g C m ⁻² h ⁻¹	F14,F15,F24	
$R_{si,l}$	nodule senescence respiration	g C m ⁻² h ⁻¹	F9,F11	
$r_{ri,l}$	root radius	m	F6b	
r_{wl}	radius of soil water films	m	F6b	
S	change in entropy	J mol ⁻¹ K ⁻¹	F2	710
T_l	soil temperature	K	F2,F8	
$U_{\chi i,l}$	uptake of nodule nonstructural C for growth	g C m ⁻² h ⁻¹	F15,F16,F24	
$V_{\chi i,l}$	nonstructural C transfer between root and nodule	g C m ⁻² h ⁻¹	F21,F24	
$V_{vi,l}$	nonstructural N transfer between root and nodule	g N m ⁻² h ⁻¹	F22,F25	
$V_{N_2i,l}$	N ₂ fixation	g N m ⁻² h ⁻¹	F12,F14,F25	
$V_{O_2maxi,l}$	O ₂ uptake by nodules under non-limiting O ₂	g O m ⁻² h ⁻¹	F4,F5,F6a	
$V_{O_2i,l}$	O ₂ uptake by nodules under ambient O ₂	g O m ⁻² h ⁻¹	F4,F6	

$V_{n,l}$	nonstructural P transfer between root and nodule	$\text{g P m}^{-2} \text{h}^{-1}$	F23,F26	
Y_n'	nodule growth yield	g C g C^{-1}	F15,F16	0.67
y	shape parameter for f_{tm}	-	F8	0.081

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