

SUPPLEMENTARY MATERIAL

Model Development

General

Ecosys is an hourly time-step model with multiple canopy and soil layers that provide a framework for simulated plant and microbial populations to acquire, transform and exchange resources (energy, water, C, N and P). The model is constructed from algorithms representing basic physical, chemical and biological processes that determine process rates in plant and microbial populations interacting within complex biomes. These algorithms interact to simulate complex ecosystem behaviour across a wide range of spatial and biological scales. The model is designed to represent terrestrial ecosystems under range of natural and anthropogenic disturbances and environmental changes at patch (spatially homogenous one-dimensional) and landscape (spatially variable two- or three-dimensional) scales. A comprehensive description of *ecosys* with a detailed listing of inputs, outputs, governing equations, parameters, results and references can be found in Grant (2001). A more detailed description of model algorithms and parameters 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 S , dissolved organic matter Q , sorbed organic matter A , microbial biomass M , and microbial residues Z , among which C, N, and P are transformed. Organic matter in litter and manure complexes are partitioned from proximate analysis results into carbohydrate, protein, cellulose, and lignin components of differing vulnerability to hydrolysis. Organic matter in POM, humus, microbial biomass and microbial residues in all complexes are also partitioned into components of differing vulnerability to hydrolysis.

The rate at which each component of each organic state in each complex is hydrolyzed during decomposition is a first-order function of the decomposer biomass M of all heterotrophic microbial populations [A1]. Decomposer biomasses are redistributed among complexes from active biomasses according to biomass – substrate concentration differences (priming) [A3]. The rate at which each component is hydrolyzed is also a Monod function of substrate concentration [A3,A5], calculated from the fraction of substrate mass colonized by M [A4]. Hydrolysis rates are controlled by T_s through an Arrhenius function [A6] and by soil water content (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 CO_2 emission from the soil surface through volatilization and diffusion. R_h may be constrained by microbial N or P concentrations, T_s , DOC and O_2 [A12 - A14]. O_2 uptake by M is driven by R_h [A16] and constrained by O_2 diffusivity to microbial surfaces [A17], as described for roots in *Autotrophic Respiration and Growth* above. Thus R_h is coupled to O_2 reduction by all aerobic M according to O_2 availability. R_h not coupled with O_2 reduction is coupled with the sequential reduction of NO_3^- , NO_2^- , and N_2O by heterotrophic denitrifiers, and with the reduction of organic C by fermenters and acetotrophic methanogens. In addition, autotrophic nitrifiers conduct NH_4^+ and NO_2^- 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 decay. M also undergoes first-order decay D_m [A23]. Internal retention and recycling of microbial N and P during decay [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,c], sensible heat flux H [B1d], and change in heat storage G) is achieved. These fluxes are controlled by aerodynamic (r_a) [B3] and canopy stomatal (r_c) [B2] resistances. Two controlling mechanisms are postulated for r_c which are solved in two successive steps:

- (1) At the leaf level, leaf resistance r_l [C4] controls gaseous 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, Autotrophic Respiration, Growth and Litterfall

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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 CO₂ 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 O₂ uptake U_{O_2} [C14b] calculated by solving for aqueous O₂ 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 Litterfall

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_r 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, C19a,b]. 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 [C19c,d]. 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. In addition, concentrations of σ_C , σ_N and σ_P in roots and mycorrhizae drive exudation of nonstructural C, N and P to DOC, DON and DOP in soil [C19e-i].

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

Root and Mycorrhizal Nutrient Uptake

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

C₄ Gross Primary Productivity

C₄ Mesophyll

In C_4 plants, the mesophyll carboxylation rate is the lesser of CO_2 - and light-limited reaction rates [C26] (Berry and Farquhar, 1978). The CO_2 -limited rate is a Michaelis-Menten function of PEP carboxylase (PEPc) activity and aqueous CO_2 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 [C10]. Leaf surface N density is controlled by leaf structural N:C and P:C ratios calculated during leaf growth from leaf non-structural N:C and P:C ratios arising from root N and P uptake (Grant, 1998) vs. 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 [C45a] is a hyperbolic function of absorbed irradiance and activity of chlorophyll associated with the bundle sheath with a quantum yield based on 3 ATP [C46]. The provision of reductant from the mesophyll to the bundle sheath in NADP-ME species is not explicitly simulated. RuBPc [C47] and chlorophyll [C48] activities are the products of specific activities and concentrations multiplied by set fractions of leaf surface N density, and from functions of C₃ product inhibition (Bowes, 1991; Stitt, 1991) [C49], ψ_c (Eq. A12 from Grant and Flanagan, 2007) and T_c [C10].

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 C_4 product transfer from the mesophyll [C37], raise C_4 product concentration in the mesophyll [C40], and slow mesophyll CO_2 fixation [C32 – C35]. This reaction sequence simulates the progressive inhibition of C_3 and C_4 carboxylation hypothesized by Sawada et al. (2002) following partial removal of C sinks in C_4 plants.

Shoot – Root - Mycorrhizal C, N, P Transfer

Shoot – root C transfers Z_{sC} are calculated such that concentrations of σ_C with respect to structural phytomass in each branch and root layer approach equilibrium according to conductances g_{sC} calculated from shoot – root distances and axis numbers in each root layer [C50] (Grant, 1998). Because σ_C is generated by CO_2 fixation in branches [C1], g_{sC} cause shoot-to-root gradients of σ_C that drive Z_{sC} . Shoot – root N and P transfers $Z_{sN,P}$ are calculated such that concentrations of $\sigma_{N,P}$ with respect to σ_C in each branch and root layer approach equilibrium according to rate constants $g_{sN,P}$ [C51]. Because $\sigma_{N,P}$ are generated by uptake in roots [C23], $g_{sN,P}$ cause root-to-shoot gradients of $\sigma_{N,P}$ that drive $Z_{sN,P}$.

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

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 and through roots in each soil layer driven by aqueous concentration gradients and dispersivities [D19] calculated from water-filled porosity [D20] and water flow length [D21].

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

Microbial Growth

Modelling the activity of symbiotic N₂ fixing bacteria in roots (e.g. *Rhizobia*) and branches (e.g. cyanobacteria) 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 or branch nodules [F1], and is constrained by temperature [F2] and microbial N or P status [F3]. Nodule respiration R in roots is constrained by the extent to which O₂ uptake meets O₂ demand [F4] imposed by respiration demand [F5]. O₂ uptake is in turn constrained by rhizosphere [O_{2r}] [F6a] which is controlled by radial diffusion of O₂ through soil water to roots and nodules [F6b]. Soil water [O₂] is maintained by dissolution of O₂ 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

N₂ fixation V_{N_2} is driven by R_g [F12], but is constrained by accumulation of nonstructural N ν_n with respect to nonstructural C and P also required for microbial growth in the root or branch nodule [F13]. Nonstructural N ν_{nd} is the product of V_{N_2} , so that [F12] simulates the inhibition of N₂ fixation by its product (Postgate, 1998). The value of V_{N_2} is also limited by the additional N needed to maintain bacterial N content $[N_n']$ of M_n [F12] (typically 1/8 that of C), so that N₂ fixation is constrained by the need of nodule bacteria for N not met from other sources (Postgate, 1998). Respiration required for N₂ fixation R_{N_2} [F14] is subtracted from R_g [F15] when calculating microbial growth [F16 – F18]. Microbial senescence drives N and P litterfall [F19 – F20].

Nodule – Root Exchange

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

Root nonstructural N (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 or branch [F22], raising v_n [F25] and hence suppressing V_{N_2} [F12 – F13]. Large v_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 v_{rt} and raise χ_{rt} , hastening the transfer of v_n from nodule to root or branch and of χ_{rt} from root or branch to nodule, lowering v_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 branch CO_2 fixation and root P uptake. All equations in Appendix F are solved for nodules in roots (i,l) and branches (i,j) except for [F6], although only those for roots are given.

Appendix G: CH₄ Production and Consumption

Anaerobic Fermenters and H₂ Producing Acetogens

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

Acetotrophic Methanogens

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

Mah, 1980). Change in $M_{i,m,j}$ is thus the difference between uptake and respiration of $A_{i,c}$, less decomposition (Eq. [G11]). This change determines $M_{i,m,a}$ used in the following calculation of $R_{i,m}$ (Eq. [G7]). Mineralization and decomposition processes are the same as those for other microbial populations.

Hydrogenotrophic Methanogens

The fermenter products CO_2 and H_2 (Eq. [G2]) are the substrates for CO_2 reduction by hydrogenotrophic methanogens ($n = h$) which are assumed to be autotrophic (Eq. [G12]). Respiration products are partitioned between CH_4 and H_2O according to Brock and Madigan (1991) (Eq. [G13]). R_h beyond that used for maintenance respiration drives the uptake of additional CO_2 (Eq. [G14]) for microbial growth according to the growth yield Y_h of hydrogenotrophic methanogenesis (Brock and Madigan, 1991) (Eq. [G15]). This growth yield is calculated by dividing the free energy change of hydrogenotrophic methanogenesis, adjusted for H_2 substrate concentration (Eq. [G16]), by the energy required to transform CO_2 into microbial C. Change in $M_{h,j}$ is thus the difference between uptake and respiration of CO_2 , less decomposition (Eq. [G17]). This change determines $M_{h,a}$ used in the following calculation of R_h (Eq. [G12]). Mineralization and decomposition processes are the same as those for other microbial populations.

Autotrophic Methanotrophs

Methane generated by acetotrophic and hydrogenotrophic methanogens is the substrate for CH_4 oxidation by autotrophic methanotrophs ($n = t$) (Eq. [G18]). The stoichiometry and energetics of the methanotrophic reactions (Eqs. [G22 – G24]) are based on those of CH_4 to CO_2 in Brock and Madigan (1991). The oxidation of CH_4 to CO_2 is coupled through an energy yield with the oxidation of CH_4 to organic C used in microbial respiration (Eq. [G19]). The energy yield from CH_4 oxidation is calculated by dividing the free energy change of CH_4 oxidation by the energy required to transform CH_4 into organic C (Eq. [G20]). Oxygen requirements to sustain CH_4 oxidation rates are then calculated from the stoichiometries of CH_4 oxidation (Eq. [G22 and G23]) and aerobic microbial respiration (Eq. [G24]). The O_2 concentrations at methanotrophic microsites are then found at which active O_2 uptake driven by requirements for CH_4 oxidation equals spherical O_2 diffusion to the microsites from the soil solution. These microsites are considered to be uniformly distributed on soil surfaces and are separated from the soil atmosphere (if present) by a water film of uniform thickness that depends upon soil water potential. The O_2 uptake by each aerobic microbial population in the model competes with that by all other aerobic microbial populations (e.g. Grant, 1995; Grant and Rochette, 1994), and is constrained by O_2 transfer rates through the gaseous and aqueous phases of the soil profile. The ratio of O_2 uptake to O_2 requirement $f_{\text{O}_2,t}$ is then used to constrain CH_4 oxidation rates (Eq. [G21]) so that CH_4 oxidation is stoichiometrically coupled to O_2 uptake. Growth respiration by methanotrophs is calculated as the difference between total respiration R_t from Eq. [G21b] and maintenance respiration $R_{m,t}$ from Eqs. [18-19] of Grant et al. (1993a). Growth respiration drives the uptake and transformation of additional CH_4 into microbial biomass $M_{t,c}$ (Eq. [G25]) according to the growth yield. This yield is calculated by dividing the free energy change of CH_4 oxidation (Brock and Madigan, 1991) (Eq. [G18]) by the energy required to construct new microbial biomass from CH_4 (Eq. [G26]). Net growth of the methanotrophic population

$M_{t,j,c}$ is calculated as the uptake of $\text{CH}_4 - \text{C}$ minus respiration and decomposition of assimilated C (Eq. [G27]). This change determines $M_{t,a}$ used in the following calculation of X'_t (Eq. [G18]). Mineralization and decomposition processes are the same as those for other microbial populations.

This submodel of autotrophic methanotrophy has been used to simulate methanotrophic growth yields, specific growth rates, CH_4 concentration profiles and the sensitivity of CH_4 uptake to temperature and water content in soil columns (Grant, 1999). The combined submodels of anaerobic fermentation, acetotrophic methanogenesis, hydrogenotrophic methanogenesis and autotrophic methanotrophy have been used to simulate methanogenic growth yields, specific growth rates, and the time course of CH_4 emissions from differently amended soil columns at different temperatures (Grant, 1998b). All input parameter values used in Eqs. [G1] to [G27] (Table 1) were derived from the microbiological literature and remain unchanged from those used in Grant (1998b) and in Grant (1999).

Appendix H: Inorganic N Transformations

Mineralization and Immobilization of Ammonium by All Microbial Populations

Each functional component j (j = labile or resistant) of each microbial population m (m = obligately aerobic bacteria, obligately aerobic fungi, facultatively anaerobic denitrifiers, anaerobic fermenters plus H_2 -producing acetogens, acetotrophic methanogens, hydrogenotrophic methanogens and methanotrophs, NH_4^+ and NO_2^- oxidizers, and non-symbiotic diazotrophs) in each substrate-microbe complex i (i = animal manure, coarse woody plant residue, fine non-woody plant residue, particulate organic matter, or humus) seeks to maintain a set C:N ratio by mineralizing NH_4^+ ([H1a]) or by immobilizing NH_4^+ ([H1b]) or NO_3^- ([H1c]). Provision is made for C:N ratios to rise above set values during immobilization, but at a cost to microbial function. These transformations control the exchange of N between organic and inorganic states.

Oxidation of DOC and Reduction of Oxygen by Heterotrophs

Constraints on heterotrophic oxidation of DOC imposed by O_2 uptake are solved in four steps:

- 1) DOC oxidation under non-limiting O_2 is calculated from active biomass and DOC concentration ([H2]),
- 2) O_2 reduction under non-limiting O_2 is calculated from 1) using a set respiratory quotient ([H3]),
- 3) O_2 reduction under ambient O_2 is calculated from radial O_2 diffusion through water films of thickness determined by soil water potential ([H4a]) coupled with active uptake at heterotroph surfaces driven by 2) ([H4b]). O_2 diffusion and active uptake is population-specific, allowing the development of more anaerobic conditions at microbial surfaces associated with more biologically active substrates. O_2 uptake by

heterotrophs also accounts for competition with O_2 uptake by nitrifiers, roots and mycorrhizae,

- 4) DOC oxidation under ambient O_2 is calculated from 2) and 3) ([H5]). The energy yield of DOC oxidation drives the uptake of additional DOC for construction of microbial biomass $M_{i,h}$ according to construction energy costs of each heterotrophic population (Eqs. [7] to [13] in Grant and Pattey, 2003). Energy costs of denitrifiers are slightly larger than those of obligate heterotrophs, placing denitrifiers at a competitive disadvantage for growth and hence DOC oxidation if electron acceptors other than O_2 are not used.

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

Constraints imposed by NO_3^- availability on DOC oxidation by denitrifiers are solved in five steps:

- 1) NO_3^- reduction under non-limiting NO_3^- is calculated from a fraction of electrons demanded by DOC oxidation but not accepted by O_2 because of diffusion limitations ([H6]),
- 2) NO_3^- reduction under ambient NO_3^- is calculated from 1) ([H7]),
- 3) NO_2^- reduction under ambient NO_2^- is calculated from demand for electrons not met by NO_3^- in 2) ([H8]),
- 4) NO_2^- reduction under ambient NO_2^- is calculated from demand for electrons not met by NO_2^- in 3) ([H9]),
- 5) additional DOC oxidation enabled by NO_x reduction in 2), 3) and 4) is added to that enabled by O_2 reduction from [H5], the energy yield of which drives additional DOC uptake for construction of $M_{i,n}$. This additional uptake offsets the disadvantage incurred by the larger construction energy costs of denitrifiers.

Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers

Constraints on nitrifier oxidation of NH_3 imposed by O_2 uptake are solved in four steps:

- 1) substrate (NH_3) oxidation under non-limiting O_2 is calculated from active biomass and from NH_3 and CO_2 concentrations ([H11]),
- 2) O_2 reduction under non-limiting O_2 is calculated from 1) using set respiratory quotients ([H12]),
- 3) O_2 reduction under ambient O_2 is calculated from radial O_2 diffusion through water films of thickness determined by soil water potential ([H13a]) coupled with active uptake at nitrifier surfaces driven by 2) ([H13b]). O_2 uptake by nitrifiers also accounts for competition with O_2 uptake by heterotrophic DOC oxidizers, roots and mycorrhizae,
- 4) NH_3 oxidation under ambient O_2 is calculated from 2) and 3) ([H14]). The energy yield of NH_3 oxidation drives the fixation of CO_2 for construction of microbial biomass $M_{i,n}$ according to construction energy costs of each nitrifier population (Eqs. [32] to [34] in Grant and Pattey, 2003).

Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers

Constraints on nitrifier oxidation of NO_2^- imposed by O_2 uptake ([H15] to [H18]) are solved in the same way as are those of NH_3 ([H11] to [H14]). The energy yield of NO_2^- oxidation drives the fixation of CO_2 for construction of microbial biomass $M_{i,o}$ according to construction energy costs of each nitrifier population.

Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers

Constraints on nitrifier oxidation imposed by NO_2^- availability are solved in three steps:

- 1) NO_2^- reduction under non-limiting NO_2^- is calculated from a fraction of electrons demanded by NH_3 oxidation but not accepted by O_2 because of diffusion limitations ([H19]),
- 2) NO_2^- reduction under ambient NO_2^- and CO_2 is calculated from step (1) ([H20]), competing for NO_2^- with [H18],
- 3) additional NH_3 oxidation enabled by NO_2^- reduction in 2) [H21] is added to that enabled by O_2 reduction from [H14]. The energy yield from this oxidation drives the fixation of additional CO_2 for construction of $M_{i,n}$.

Appendix A: Microbial C, N and P Transformations

Decomposition

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

$$D_{Si,j,l,N,P} = D_{Si,j,l,C} (S_{i,j,l,N,P} / S_{i,j,l,C})$$

$$D_{Zi,j,l,N,P} = D_{Zi,j,l,C} (Z_{i,j,l,N,P} / Z_{i,j,l,C})$$

$$D_{Ai,l,N,P} = D_{Ai,l,C} (A_{i,l,N,P} / A_{i,l,C})$$

$$Y_{i,l,C} = k_{ts} (G_{i,l,C} F_s [Q_{i,l,C}]^b - X_{i,l,C})$$

$$Y_{i,l,N,P} = Y_{i,l,C} (Q_{i,l,N,P} / Q_{i,l,C})$$

$$Y_{i,l,N,P} = Y_{i,l,C} (X_{i,l,N,P} / X_{i,l,C})$$

decomposition of N and P are [A7a]

driven by that of C in litter, POC,
humus, microbial residues [A7b]
and adsorbed SOC [A7c]

Freundlich sorption of DOC [A8]

($Y_{i,l,C} > 0$) adsorption of [A9]
DON, DOP

($Y_{i,l,C} < 0$) desorption of [A10]
DON, DOP

Microbial Growth

$$R_h = \sum_i \sum_n \sum_l R_{hi,n,l}$$

$$R_{hi,n,l} = R'_{hn} \min \{ C_{Ni,n,l,a} / C_{Nj}, C_{Pi,n,l,a} / C_{Pj} \}$$

$$R'_{hi,n,l} = M_{i,n,a,l,C} \{ R_{hi,n,l} [Q_{i,l,C}] \} / \{ (K_m Q_C + [Q_{i,l,C}]) \} f_{igl} f_{\psi gl}$$

$$R_{hi,n,l} = R'_{hi,n,l} (U_{O2i,n,l} / U'_{O2i,n,l})$$

$$f_{\psi gl} = 1.0 - 6.67 (1.0 - e^{(M \psi_s / (R T_s l))})$$

$$U'_{O2i,n,l} = 2.67 R'_{hi,n,l}$$

$$U_{O2i,n,l} = U'_{O2i,n,l} [O_{2mi,n,l}] / ([O_{2mi,n,l}] + K_{O_2})$$

$$= 4 \pi \bar{n} M_{i,n,a,l,C} D_{sO2l} [r_m r_{wl} / (r_{wl} - r_m)] ([O_{2sl}] - [O_{2mi,n,l}])$$

$$R_{mi,n,j,l} = R_m M_{i,n,j,l,N} f_{tml}$$

$$f_{tml} = e^{[y (T_{sl} - 298.16)]}$$

$$R_{gi,n,l} = R_{hi,n,l} - \sum_j R_{mi,n,j,l}$$

$$U_{i,n,l,C} = \min (R_{hi,n,l}, \sum_j R_{mi,n,j,l}) + R_{gi,n,l} (1 + \Delta G_x / E_m)$$

total heterotrophic respiration [A11]

R_h constrained by microbial N, P [A12]

R_h constrained by substrate DOC, [A13]
 T_s and ψ

R_h constrained by O_2 [A14]

ψ_s constraints on microbial growth [A15]

O_2 demand driven by potential R_h [A16]

active uptake coupled with radial [A17a]
diffusion of O_2 [A17b]

maintenance respiration [A18]

temperature sensitivity of R_m [A19]

growth respiration [A20]

DOC uptake driven by R_g [A21]

$$U_{i,n,lN,P} = U_{i,n,l} Q_{i,lN,P} / Q_{i,l,C}$$

$$D_{Mi,n,j,l,C} = D_{Mi,j} M_{i,n,j,l,C}$$

$$D_{Mi,n,j,N,P} = D_{Mi,j} M_{i,n,j,l,N,P} f_{di,n,lN,P}$$

$$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,lC} \square F_j R_{hi,n,l} - D_{Mi,n,j,l,C}$$

$$\delta M_{i,n,j,l,C} / \delta t = F_j U_{i,n,lC} \square R_{mi,n,j,l} - D_{Mi,n,j,l,C}$$

Microbial Nutrient Exchange

$$U_{NH4i,n,j,l} = (M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N})$$

$$U_{NH4i,n,j,l} = \min \{ (M_{i,n,j,l,C} C_{Nj} - M_{i,n,j,l,N}), \\ U'_{NH4} a_{i,n,j,l} ([NH_4^{\square}_{i,n,j,l}] - [NH_4^{\square}_{mn}]) / ([NH_4^{\square}_{i,n,j,l}] - [NH_4^{\square}_{mn}] + K_{NH4}) \}$$

$$U_{NO3i,n,j,l} = \min \{ (M_{i,n,j,l,C} C_{Nj} - (M_{i,n,j,l,N} + U_{NH4i,n,j,l})), \\ U'_{NO3} a_{i,n,j,l} ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}]) / ([NO_3^-_{i,n,j,l}] - [NO_3^-_{mn}] + K_{NO3}) \}$$

$$U_{PO4i,n,j,l} = (M_{i,n,j,l,C} C_{Pj} - M_{i,n,j,l,P})$$

$$U_{PO4i,n,j,l} = \min \{ (M_{i,n,j,l,C} C_{Pj} - M_{i,n,j,l,P}), \\ U'_{PO4} a_{i,n,j,l} ([H_2PO_4^-_{i,n,j,l}] - [H_2PO_4^-_{mn}]) / ([H_2PO_4^-_{i,n,j,l}] - [H_2PO_4^-_{mn}] + K_{PO4}) \}$$

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

$$R_{\Phi_{i,n=fj,l}} \square E_{\Phi} \Phi_{i,n=fj,l} \square$$

$$\delta M_{i,n,j,l,N} / \delta t = F_j U_{i,n,l,N} + U_{NH4i,n,j,l} + U_{NO3i,n,j,l} + \Phi_{i,n=fj,l} - D_{Mi,n,j,l,N}$$

$$\delta M_{i,n,j,l,P} / \delta t = F_j U_{i,n,l,P} + U_{PO4i,n,j,l} - D_{Mi,n,j,l,P}$$

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

$$\text{DON, DOP uptake driven by } U_{i,n,lC} \quad [A22]$$

$$\text{first-order decay of microbial C,} \quad [A23]$$

$$\text{decay of microbial N, P} \quad [A24]$$

$$[R_{hi,n,l} > R_{mi,n,j,l}] \quad \text{microbial growth} \quad [A25a]$$

$$[R_{hi,n,l} < R_{mi,n,j,l}] \quad \text{microbial senescence} \quad [A25b]$$

$$U_{NH4} < 0 \quad \text{net mineralization} \quad [A26a]$$

$$U_{NH4} > 0 \quad \text{net immobilization} \quad [A26b]$$

$$U_{NO3} > 0 \quad \text{net immobilization} \quad [A26c]$$

$$U_{PO4} < 0 \quad \text{net mineralization} \quad [A26d]$$

$$U_{PO4} > 0 \quad \text{net immobilization} \quad [A26e]$$

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

$$\text{diazotrophic population} \quad [A28]$$

$$\text{respiration needed to drive N}_2 \text{ fixation} \quad [A28]$$

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

$$\text{active microbial biomass} \quad [A30a]$$

$$\text{calculated from labile fraction}$$

Humification

$H_{Si,j=\text{lignin},l,C} = D_{Si,j=\text{lignin},l,C}$	decomposition products of litter	[A31]
$H_{Si,j=\text{lignin},l,N,P} = D_{Si,j=\text{lignin},l,N,P}$	substrate added to POC depending on lignin	[A32]
$H_{Si,j\neq\text{lignin},l,C} = H_{Si,j=\text{lignin},l,C} \mathbf{L}_{hj}$		[A33]
$H_{Si,j\neq\text{lignin},l,N,P} = H_{Si,j\neq\text{lignin},l,C} S_{i,l,N,P} / S_{i,l,C}$		[A34]
$H_{Mi,n,j,l,C} = D_{Mi,n,j,l,C} \mathbf{F}_{\mathbf{h}}$	fraction of microbial decay products added to humus	[A35]
$H_{Mi,n,j,l,N,P} = H_{Mi,n,j,l,C} M_{i,n,j,l,N,P} / M_{i,n,j,l,C}$		[A36]
$\mathbf{F}_{\mathbf{h}} = 0.167 + 0.167 F_{\text{clay}} + 0.167 \times 10^{-6} G_{i,l,C}$	fraction of D_M added to humus depends on clay and SOC	[A37]
$H_{Zi,n,j,l,C} = D_{Mi,n,j,l,C} - H_{Mi,n,j,l,C}$	remainder of microbial decay products added to microbial	[A38]
$H_{Zi,n,j,l,N,P} = D_{Mi,n,j,l,N,P} - H_{Mi,n,j,l,N,P}$	residues	[A39]

Definition of Variables in Appendix A

Variable	Definition	Unit	Equation	Value	Reference
<i>subscripts</i>					
i	substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus				
j	kinetic component: labile l , resistant r , active a				
l	soil or litter layer				
n	microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)				
<i>variables</i>					
$A_{i,l,C}$	mass of adsorbed SOC	g C m ⁻²	[A1c,A2c]		
$[A_{i,l,C}]$	concentration of adsorbed SOC in soil	g C Mg ⁻¹	[A4c]		
a	microbial surface area	m ² m ⁻²	[A26]		
B	parameter such that $f_{ig} = 1.0$ at $T_l = 298.15$ K		[A6]	26.235	
b	Freundlich exponent for sorption isotherm		[A8]	0.85	Grant et al. (1993a,b)
β	specific colonization rate of uncolonized substrate	-	[A5]	2.5	Grant et al. (2010)
$C_{N,Pi,n,a,l}$	ratio of $M_{i,n,a,N,P}$ to $M_{i,n,a,C}$	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 = labile and resistant, respectively	Grant et al. (1993a,b)
$D_{Ai,l,C}$	decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ producing Q in [A13]	g C m ⁻² h ⁻¹	[A1c,A7c,A31c]		
$D_{Aj,C}$	specific decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ at 25°C and saturating[$A_{i,l,C}$]	g C g C ⁻¹ h ⁻¹	[A4c]	0.025	Grant et al. (1993a,b)
$D_{Ai,j,l,N,P}$	decomposition rate of $A_{i,l,N,P}$ by $M_{i,d,l,C}$	g N or P m ⁻² h ⁻¹	[A7c]		
$D'_{Ai,j,l,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C ⁻¹ h ⁻¹	[A1a,A4c]		
D_{Mij}	specific decomposition rate of $M_{i,n,j}$ at 30°C	g C g C ⁻¹ h ⁻¹	[A23,A24]	1.6 x 10 ⁻³ and 8.0 x 10 ⁻⁵ for j = labile and resistant, respectively	Grant et al. (1993a,b)
$D_{M_{i,n,j,l,C}}$	decomposition rate of $M_{i,n,j,l,C}$	g C m ⁻² h ⁻¹	[A23,A25,A35,A 38]		
$D_{M_{i,n,j,l,N,P}}$	decomposition rate of $M_{i,n,j,l,N,P}$	g N or P m ⁻² h ⁻¹	[A24,A29,A39]		
$D_{S_{i,j,l,C}}$	decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing Q in [A13]	g C m ⁻² h ⁻¹	[A1a,A7a,A31a]		
$D_{Sj,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating [$S_{i,l,C}$]	g C g C ⁻¹ h ⁻¹	[A4a]	1.0, 1.0, 0.15, and 0.025 for j = protein, carbohydrate, cellulose, and lignin, 0.009 for POC, and 0.009 and 0.003 for active and passive humus.	Grant et al. (1993a,b)
$D_{S_{i,j,l,N,P}}$	decomposition rate of $S_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m ⁻² h ⁻¹	[A7a, A32]		

$D'_{Si,j,l,C}$	specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C ⁻¹ h ⁻¹	[A1a,A4a]		
D_{sO_2l}	aqueous dispersivity–diffusivity of O ₂ during microbial uptake in soil	m ² h ⁻¹	[A17]		
$D_{Zi,j,l,C}$	decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing Q in [A13]	g C m ⁻² h ⁻¹	[A1b,A7b]		
$D_{Zi,j,l,N,P}$	decomposition rate of $Z_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m ⁻² h ⁻¹	[A7b]		
$D_{Zj,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[$Z_{i,l,C}$]	g C g C ⁻¹ h ⁻¹	[A4b]	0.25 and 0.05 for j = labile and resistant biomass	Grant et al. (1993a,b)
$D'_{Zi,j,l,C}$	specific decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C ⁻¹ h ⁻¹	[A1b,A4b]		
ΔG_x	energy yield of C oxidation with different reductants x	kJ g C ⁻¹	[A21]	37.5 (x = O ₂), 4.43 (x = DOC)	
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_{clay}	fraction of mineral soil as clay	Mg Mg ⁻¹	[A37]		
F_h	fraction of products from microbial decomposition that are humified (function of clay content)		[A35, A37]		Sørensen (1981)
F_l	fraction of microbial growth allocated to labile component $M_{i,n,l}$		[A25,A29,A30]	0.55	Grant et al. (1993a,b)
F_r	fraction of microbial growth allocated to resistant component $M_{i,n,r}$		[A25,A29,A30]	0.45	Grant et al. (1993a,b)
F_s	equilibrium ratio between $Q_{i,l,C}$ and $H_{i,l,C}$		[A8]		
$f_{di,n,N,P}$	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 $U_{\text{PO}_4} < 0$	
$f_{\text{ig}l}$	temperature function for microbial growth respiration	dimensionless	[A1,A6,A13]		

f_{uml}	temperature function for maintenance respiration	dimensionless	[A18,A19]		
$f_{\psi_{\text{gl}}}$	soil water potential function for microbial, root or mycorrhizal growth respiration	dimensionless	[A13,A15]		Pirt (1975)
$\Phi_{i,n=f,j,l}$	non-symbiotic N ₂ fixation by heterotrophic diazotrophs ($n=f$)	g N m ⁻² h ⁻¹	[A27,A28,A29]		
$G_{i,l,C}$	total C in substrate-microbe complex	g C Mg ⁻¹	[A1,A2c,A3a,A8,A37]		
[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]	195 x 10 ³	
$H_{M_{i,n,j,l,C}}$	transfer of microbial C decomposition products to humus	g C m m ⁻² h ⁻¹	[A35,A36,A38]		
$H_{M_{i,n,j,l,N,P}}$	transfer of microbial N or P decomposition products to humus	g N or P m ⁻² h ⁻¹	[A36,A39]		
$H_{S_{i,j,l,C}}$	transfer of C hydrolysis products to particulate OM	g C m ⁻² h ⁻¹	[A31,A32,A33,A34]		
$H_{S_{i,j,l,N,P}}$	transfer of N or P hydrolysis products to particulate OM	g N or P m ⁻² h ⁻¹	[A32,A34]		
$H_{Z_{i,n,j,l,C}}$	transfer of microbial C decomposition products to microbial residue	g C m m ⁻² h ⁻¹	[A38]		
$H_{Z_{i,n,j,l,N,P}}$	transfer of microbial N or P decomposition products to microbial residue	g N or P m ⁻² h ⁻¹	[A39]		
K_{IS}	inhibition constant for microbial colonization of substrate	-	[A5]	0.5	Grant et al. (2010)
K_{NH_4}	M-M constant for NH ₄ ⁺ uptake at microbial surfaces	g N m ⁻³	[A26]	0.40	
K_{NO_3}	M-M constant for NO ₃ ⁻ uptake at microbial surfaces	g N m ⁻³	[A26]	0.35	
K_{PO_4}	M-M constant for H ₂ PO 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	[A4]	25	Grant et al.

K_{mD}	Michaelis–Menten constant for $D_{Sij,C}$	g C Mg^{-1}	[A4]	75	(1993a,b); Lizama and Suzuki (1990)
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_{2s} by microbes, roots and mycorrhizae	$\text{g O}_2 \text{ m}^{-3}$	[A17]	0.32	Griffin (1972)
k_{ts}	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	
$M_{i,d,l,C}$	heterotrophic microbial C used for decomposition	g C m^{-2}	[A1,A3a,A4]		
$M_{i,n,j,l,C}$	microbial C	g C m^{-2}	[A13,A17A23,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 $G_{i,l,C}$	g C m^{-2}	[A3,A13,A17, A30]		
$[M_{i,n,a,l,C}]$	concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,l,C} / \theta_l$	g C m^{-3}	[A3, A5]		
n	number of microbial microsites	m^{-2}	[A17b]		
$[\text{NH}_4^+_{i,n,j,l}]$	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 NH_4^+ 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 microsites	$\text{g O}_2 \text{ m}^{-3}$	[A17]		
$[\text{O}_{2sl}]$	O_2 concentration in soil solution	$\text{g O}_2 \text{ m}^{-3}$	[A17]		
$Q_{i,l,C}$	DOC from products of $D_{\text{Si},j,l,C}$ [A3] and $D_{\text{Zi},j,l,C}$ [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]		
$Q_{i,l,N,P}$	DON and DOP from products of $(D_{\text{Si},j,l,N,P} + D_{\text{Zi},j,l,N,P})$	g N or P m^{-2}	[A9,A22]		
q_m	rate constant for reallocating $M_{i,a,l,C}$ to $M_{i,d,l,C}$	h^{-1}	[A3a]	0.5	
R	gas constant	$\text{J mol}^{-1} \text{ K}^{-1}$	[A6,A15,C10]	8.3143	
$R_{\phi i,n=f,j,l}$	respiration for non-symbiotic 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	$\text{g C m}^{-2} \text{ h}^{-1}$	[A5,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	$\text{g C g C}^{-1} \text{ h}^{-1}$	[A12]	0.125	Shields et al. (1973)
$R'_{hi,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2 and ambient DOC, nutrients, θ and temperature	$\text{g C m}^{-2} \text{ h}^{-1}$	[A13,A14,A16]		
R_m	specific maintenance respiration at 25°C	$\text{g C g N}^{-1} \text{ h}^{-1}$	[A18]	0.0115	Barnes et al. (1998)

$R_{m,i,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[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	$\text{J mol}^{-1} \text{ K}^{-1}$	[A6,C10]	710	Sharpe and DeMichelle (1977)
$[S_{ij,l,C}]$	concentration of $S_{ij,l,C}$ in soil	g C Mg^{-1}	[A4a]		
$S_{ij,l,C}$	mass of colonized litter, POC or humus C	g C m^{-2}	[A2a,A5,A7a,A33]		
$S'_{ij,l,C}$	mass of uncolonized litter, POC or humus C	g C m^{-2}	[A5]		
$S_{ij,l,N,P}$	mass of litter, POC or humus N or P	g N or P m^{-2}	[A7a,A33]		
T_{sl}	soil temperature	K	[A6,A15.A19]		
$U_{i,n,C}$	uptake of $Q_{i,l,C}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	$\text{g C m}^{-2} \text{ h}^{-1}$	[A5,A21,A22,A25]		
$U_{i,n,N,P}$	uptake of $Q_{i,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	$\text{g N or P m}^{-2} \text{ h}^{-1}$	[A22,A29]		
$U_{\text{NH}_4,i,n,j,l}$	NH_4^+ uptake by microbes	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26, A27,A29]		
U'_{NH_4}	maximum U_{NH_4} at 25 °C and non-limiting NH_4^+	$\text{g N m}^{-2} \text{ h}^{-1}$	[A26]	5.0×10^{-3}	
$U_{\text{NO}_3,i,n,j,l}$	NO_3^- uptake by microbes	$\text{g N m}^{-2} \text{ h}^{-1}$	[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}	
$U_{\text{O}_2,i,n}$	O_2 uptake by $M_{i,n,a,l}$ under ambient O_2	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A17]		
$U'_{\text{O}_2,i,n}$	O_2 uptake by $M_{i,n,a,l}$ under nonlimiting O_2	$\text{g m}^{-2} \text{ h}^{-1}$	[A14,A16,A17]		

$U_{PO4i,n,j,l}$	H ₂ PO ₄ ⁻ uptake by microbes	g N m ⁻² h ⁻¹	[A26,A27,A29]	
U'_{PO4}	maximum U_{PO4} at 25 °C and non-limiting H ₂ PO ₄ ⁻	g N m ⁻² h ⁻¹	[A26]	5.0 x 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	g C m ⁻² h ⁻¹	[A8,A9,A10]	
$Y_{i,l,N,P}$	sorption of N or P hydrolysis products	g P m ⁻² h ⁻¹	[A9,A10]	
$[Z_{ij,l,C}]$	concentration of $Z_{ij,l,C}$ in soil	g C Mg ⁻¹	[A4b]	
$Z_{ij,l,C}$	mass of microbial residue C in soil	g C m ⁻²	[A2b,A7b]	
$Z_{ij,l,N,P}$	mass of microbial residue N or P in soil	g P m ⁻²	[A7b]	

Appendix B: Soil-Plant Water Relations

Canopy Transpiration

$Rn_{ci} + LE_{ci} + H_{ci} + G_{ci} = 0$	canopy energy balance	[B1a]
$LE_{ci} = L (e_a - e_{ci}(T_{ci}, \psi_{ci})) / r_{ai}$	LE from canopy evaporation	[B1b]
$LE_{ci} = L (e_a - e_{ci}(T_{ci}, \psi_{ci})) / (r_{ai} + r_{ci}) - LE_{ci}$ from [B1b]	LE from canopy transpiration	[B1c]
$H_{ci} = \rho C_p (T_a - T_{ci}) / r_{ai}$	H from canopy energy balance	[B1d]
$r_{cmini} = 0.64 (C_b - C_i') / V_c' i$	r_c driven by rates of carboxylation vs. diffusion	[B2a]
$r_{ci} = r_{cmini} + (r_{cmaxi} - r_{cmini}) e^{(-\beta \psi_{ci})}$	r_c constrained by water status	[B2b]
$r_{ai} = \{(\ln((z_u - z_{di}) / z_{ri})^2 / (K^2 u_a))\} / (1 - 10 Ri)$	r_a driven by windspeed, surface	[B3a]
$Ri = \{g (z_u - z_{ri}) / (u_a^2 T_a)\} (T_a - T_c)$	r_a adjusted for stability vs. buoyancy	[B3b]
$\psi_{ti} = \psi_{ci} - \psi_{pi}$		[B4]

Root and Mycorrhizal Water Uptake

$U_{wi} = \sum_l \sum_r U_{wi,r,l}$		[B5]
$U_{wi,r,l} = (\psi_c' i - \psi_s' l) / (\mathcal{Q}_{si,r,l} + \mathcal{Q}_{ri,r,l} + \sum_x \mathcal{Q}_{ai,r,l,x})$	U_w along hydraulic gradient	[B6]
$\psi_c' i = \psi_{ci} + 0.01 z_{bi}$		[B7]
$\psi_s' l = \psi_{sl} - 0.01 z_l$		[B8]
$\mathcal{Q}_{si,r,l} = \ln\{(d_{i,r,l} / r_{i,r,l}) / (2\pi L_{i,r,l} \kappa_{ri,r,l})\} \theta_{wl} / \theta_{pl}$		[B9]

$$\Omega_{i,r,l} = \Omega_{i,r,l} / L_{i,r,l} \quad [B10]$$

$$\Omega_{ai,r,l,x=1} = \Omega_{ai,r,l} / \{n_{i,r,l,1} (r_{i,r,l,1} / r'_{i,r})^4\} + \gamma \Omega_{ai,r,l} / \{n_{i,r,l,1} (r_{bi} / r'_{bi})^4\} \Sigma_{i,r,l} (M_{i,r,l}) / M_{i,r,l} \quad [B11]$$

$$\Omega_{ai,r,l,x=2} = \Omega_{ai,r,l} (L_{i,r,l,2} / n_{i,r,l,2}) / \{n_{i,r,l,2} (r_{i,r,l,2} / r'_{i,r})^4\} \quad [B12]$$

$$\delta L_{i,r,l,1} / \delta t = \delta M_{i,r,l,1} / \delta t \nu_r \{ \rho_r (1 - \theta_{p_{i,r}}) (\pi r_{i,r,l,1}^2) \} \quad [B13]$$

Canopy Water Potential

$$(e_a - e_{i(T_{ci})}) / (r_{ai} + r_{ci}) [B1] = \Sigma_l \Sigma_r (\psi_{ci} - \psi_{si}) / (\Omega_{si,r,l} + \Omega_{ci,r,l} + \Sigma_x \Omega_{ai,r,l,x}) + X_{ci} \delta \psi_{ci} / \delta t$$

[B14]

ψ_{ci} 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)				

r	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	mol mol ⁻¹	[B2,C2,C5]		
C'_{ci}	[CO ₂] in canopy leaves at $\psi_{ci} = 0$ MPa	mol mol ⁻¹	[B2]	0.70 C_b	Larcher (2001)
$d_{i,r,l}$	half distance between adjacent roots	m	[B9]		
E_{ci}	canopy transpiration	m ³ m ⁻² h ⁻¹	[B1,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]		
G_{ci}	canopy storage heat flux	W m ⁻²	[B1]		
H_{ci}	canopy sensible heat flux	W m ⁻²	[B1]		
K	von Karman's constant		[B3a]	0.41	
$\kappa_{i,r,l}$	hydraulic conductivity between soil and root surface	m ² MPa ⁻¹ h ⁻¹	[B9]		
γ	scaling factor for bole axial resistance from primary root axial resistance	-	[B11]	1.6 x 10 ⁴	Grant et al. (2007)
L	latent heat of evaporation	J g ⁻¹	[B1]	2460	
LE_{ci}	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 x 10 ⁹ deciduous 1.0 x 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 x 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	m ³ m ⁻³	[B9]		
θ_{pl}	soil porosity	m ³ m ⁻³	[B9]		
$\theta_{pi,r}$	root porosity	m ³ m ⁻³	[B13]		
Ri	Richarson number		[B3a,B3b]		van Bavel and Hillel (1976)
Rn_{ci}	canopy net radiation	W m ⁻²	[B1]		
r_{ai}	aerodynamic resistance to vapor flux from canopy	s m ⁻¹	[B1,B3a]		
r_{bi}	radius of bole at ambient ψ_{ci}	m	[B11]		
r_{bi}'	radius of bole at $\psi_{ci} = 0$ 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 x 10 ³	Larcher (2001)
r_{cmini}	minimum r_{ci} at $\psi_{ci} = 0$ 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 $\psi_{ti,l,z}$	m	[B9,B11,B12,B13]		

$r'_{i,r}$	radius of secondary roots or mycorrhizae at $\psi_{i,l,z} = 0$ MPa	m	[B11,B12]	2.0 x 10 ⁻⁴ tree 1.0 x 10 ⁻⁴ bush 0.05 x 10 ⁻⁴ mycorrhizae	
ρ_r	root specific density	g C g FW ⁻¹	[B13]	0.05	Grant (1998)
T_a	air temperature	K	[B3b]		
T_c	canopy temperature	K	[B3b]		
U_{wi}	total water uptake from all rooted soil layers	m ³ m ⁻² h ⁻¹	[B5,B14]		
$U_{wi,r,l}$	water uptake by root and mycorrhizal surfaces in each soil layer	m ³ m ⁻² h ⁻¹	[B5,B6]		
u_a	wind speed measured at z_u	m s ⁻¹	[B3a,B3b]		
V'_c	potential canopy CO ₂ fixation rate at $\psi_{c,i} = 0$ MPa	μmol m ⁻² s ⁻¹	[B2]		
v_r	root specific volume	m ³ g FW ⁻¹ μ	[B13]	10 ⁻⁶	Grant (1998)
X_{ci}	canopy capacitance	m ³ m ⁻² MPa ⁻¹	[B14]		
ψ_{ci}	canopy water potential	MPa	[B4,B7,B14]		
$\psi'_{c,i} \square$	$\psi_{ci} +$ canopy gravitational potential \square	MPa	[B6,B7]		
$\psi_{\pi i} \square$	canopy osmotic potential	MPa	[B4]		
$\psi_{sl} \square$	soil water potential	MPa	[B8]		
$\psi'_{s,i} \square$	$\psi_{sl} +$ soil gravitational potential \square	MPa	[B6,B8]		
ψ_{ti}	canopy turgor potential	MPa	[B2b,B4]	1.25 at $\psi_c = 0$	
$z_{bi} \square$	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, Autotrophic Respiration, Growth and Litterfall

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]
$V_{gi,j,k,l,m,n,o} = (C_b - C_{ii,j,k,l,m,n,o}) / r_{li,j,k,l,m,n,o}$	$V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}$ diffusion	[C2]
$V_{ci,j,k,l,m,n,o} = \min\{V_{bi,j,k,l,m,n,o}, V_{ji,j,k,l,m,n,o}\}$	carboxylation	[C3]
$r_{li,j,k,l,m,n,o} = r_{mini,j,k,l,m,n,o} + (r_{maxi} - r_{mini,j,k,l,m,n,o}) e^{(-\beta_{li} \psi_{li})}$	r_l is leaf-level equivalent of r_c	[C4]
$r_{mini,j,k,l,m,n,o} = (C_b - C_i') / V_{ci,j,k,l,m,n,o}$	minimum r_l is driven by carboxylation	[C5]
$V_{bi,j,k,l,m,n,o} = V_{bmax,i,j,k} (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (C_{ci,j,k,l,m,n,o} + K_{ci}) f_{\psi_{i,j,k,l,m,n,o}}$	CO ₂ and water f_{ψ} constraints on V_b	[C6a]
$V_{bmax,i,j,k} = V_{b'} F_{rubisco_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{bi} f_{ci}$	temperature f_{tb} and nutrient f_{ic} constraints on V_{bmax}	[C6b]
$\Gamma_{i,j,k} = 0.5 O_c V_{max,i,j,k} K_{ci} / (V_{bmax,i,j,k} K_{oi})$	CO ₂ compensation point	[C6c]
$V_{max,i,j,k} = V_o' F_{rubisco_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{toi}$	oxygenation	[C6d]
$K_{ci} = K_{ci} f_{tkci} (1 + O_c / (K_{oi} f_{tkoi}))$	M-M constant for V_b	[C6e]
$V_{ji,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o} Y_{i,j,k,l,m,n,o} f_{\psi_{i,j,k,l,m,n,o}}$	water constraints on V_j	[C7a]
$Y_{i,j,k,l,m,n,o} = (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (4.5 C_{ci,j,k,l,m,n,o} + 10.5 \Gamma_{i,j,k})$	carboxylation efficiency of V_j	[C7b]
$J_{i,j,k,l,m,n,o} = (\epsilon I_{i,l,m,n,o} + J_{max,i,j,k} - ((\epsilon I_{i,l,m,n,o} + J_{max,i,j,k})^2 - 4\alpha\epsilon I_{i,l,m,n,o} J_{max,i,j,k})^{0.5}) / (2\alpha)$	irradiance constraints on J	[C8a]
$J_{max,i,j,k} = V_j' F_{chlorophyll_i} M_{L_{i,j,k,prot}} / A_{i,j,k} f_{ji} f_{ci}$	temperature and nutrient constraints on J_{max}	[C8b]
$f_{\psi_{i,j,k,l,m,n,o}} = (r_{min,i,j,k,l,m,n,o} / r_{li,j,k,l,m,n,o})^{0.5}$	non-stomatal effect related to stomatal effect	[C9]

$$f_{\text{tbi}} = \exp[\mathbf{B_v} - \mathbf{H_{av}} / (RT_{\text{ci}})] / \{1 + \exp[(\mathbf{H_{dl}} - ST_{\text{ci}}) / (RT_{\text{ci}})] + \exp[(ST_{\text{ci}} - \mathbf{H_{dh}}) / (RT_{\text{ci}})]\}$$

Arrhenius functions for [C10a]

$$f_{\text{toi}} = \exp[\mathbf{B_o} - \mathbf{H_{ao}} / (RT_{\text{ci}})] / \{1 + \exp[(\mathbf{H_{dl}} - ST_{\text{ci}}) / (RT_{\text{ci}})] + \exp[(ST_{\text{ci}} - \mathbf{H_{dh}}) / (RT_{\text{ci}})]\}$$

carboxylation, oxygenation and [C10b]

$$f_{\text{tji}} = \exp[\mathbf{B_j} - \mathbf{H_{aj}} / (RT_{\text{ci}})] / \{1 + \exp[(\mathbf{H_{dl}} - ST_{\text{ci}}) / (RT_{\text{ci}})] + \exp[(ST_{\text{ci}} - \mathbf{H_{dh}}) / (RT_{\text{ci}})]\}$$

electron transport [C10c]

$$f_{\text{tkci}} = \exp[\mathbf{B_{kc}} - \mathbf{H_{akc}} / (RT_{\text{ci}})]$$

[C10d]

$$f_{\text{tkoi}} = \exp[\mathbf{B_{ko}} - \mathbf{H_{ako}} / (RT_{\text{ci}})]$$

[C10e]

$$f_{\text{ici}} = \min\{\sigma_{\text{Ni},j} / (\sigma_{\text{Ni},j} + \sigma_{\text{Ci},j} / \mathbf{KiC_N}), \sigma_{\text{Pi},j} / (\sigma_{\text{Pi},j} + \sigma_{\text{Ci},j} / \mathbf{KiC_P})\}$$

control of σ_{N} and σ_{P} vs. σ_{C} in [C11]

shoots on V_{b} , V_{j} through product inhibition and on leaf protein growth through leaf structural C:N:P ratios

$$\delta M_{\text{L}_{\text{Rij},k}} / \delta t = \delta M_{\text{L}_{\text{ij},k}} / \delta t \min\{[N'_{\text{leaf}} + (\mathbf{N_{leaf}} - N'_{\text{leaf}}) f_{\text{ici}}] / \mathbf{N_{prot}}, [\mathbf{P'_{leaf}} + (\mathbf{P_{leaf}} - \mathbf{P'_{leaf}}) f_{\text{ici}}] / \mathbf{P_{prot}}\}$$

growth of remobilizable leaf protein C [C12]

Autotrophic Respiration

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

total autotrophic respiration [C13]

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

O₂ constraint on root respiration [C14a]

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

from active uptake coupled with [C14b]

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

diffusion of O₂ from soil as for [C14c]

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

and from active uptake coupled with diffusion of O₂ from roots [C14d]

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

[C14e]

$R_{si,j} = -\min\{0.0, R_{ci,j} - R_{mi,j}\}$	remobilization in branches, roots and mycorrhizae when $R_m > R_c$	[C15]
$R_{si,r,l} = -\min\{0.0, R_{ci,r,l} - R_{mi,r,l}\}$		
$R_{mi,j} = \sum_z (N_{i,j,z} \mathbf{R}_m' f_{mi})$	maintenance respiration of branches, roots and mycorrhizae	[C16]
$R_{mi,r,l} = \sum_z (N_{i,r,l,z} \mathbf{R}_m' f_{mi})$		
$R_{gi,j} = \max\{0.0, \min\{(R_{ci,j} - R_{mi,j}) \min\{1.0, \max\{0.0, \psi_{ti} - \psi_{t'}\}\}$	growth respiration of branches, roots and mycorrhizae when $R_m < R_c$	[C17]
$R_{gi,r,l} = \max\{0.0, \min\{(R_{ci,r,l} - R_{mi,r,l}) \min\{1.0, \max\{0.0, \psi_{ti,l} - \psi_{t'}\}\}$		

Growth and Litterfall

$l_{i,j,z,C} = R_{si,j} M_{L_N^{i,j}} / M_{L_R^{i,j}}$	senescence drives litterfall of non-remobilizable material	[C18]
$l_{i,j,z,N} = l_{i,j,z,C} \mathbf{N}_{prot} (1.0 - \mathbf{X}_{mx} f_{\lambda N_{i,j}})$	litterfall of N and P is driven by that of C but reduced by	[C19a]
$l_{i,j,z,P} = l_{i,j,z,C} \mathbf{P}_{prot} (1.0 - \mathbf{X}_{mx} f_{\lambda P_{i,j}})$	translocation of remobilizabls N and P to σ_N and σ_P according to ratios of σ_N and σ_P with σ_C . root and mycorrhizal litterfall (i, r, l) calculated as for branch litterfall (i, j, z)	[C19b]
$f_{\lambda N_{i,j}} = \sigma_{C_{i,j}} / (\sigma_{C_{i,j}} + \sigma_{N_{i,j}} / \mathbf{K}_{\lambda N})$		[C19c]
$f_{\lambda P_{i,j}} = \sigma_{C_{i,j}} / (\sigma_{C_{i,j}} + \sigma_{P_{i,j}} / \mathbf{K}_{\lambda P})$		[C19d]
$x_{i,r,l,C} = r_x \sigma_{C_{i,r,l}}$		[C19e]
$x_{i,r,l,N} = r_x \sigma_{N_{i,r,l}} f_{x_{i,r,l,N}}$	root and mycorrhizal exudation driven by σ_C , σ_N and σ_P , and by $\sigma_C : \sigma_N$ and $\sigma_C : \sigma_P$.	[C19f]
$x_{i,r,l,P} = r_x \sigma_{P_{i,r,l}} f_{x_{i,r,l,P}}$		[C19g]
$f_{x_{i,r,l,N}} = \sigma_{N_{i,j}} / (\sigma_{N_{i,j}} + \sigma_{C_{i,j}} / \mathbf{K}_{xN})$		[C19h]
$f_{x_{i,r,l,P}} = \sigma_{P_{i,j}} / (\sigma_{P_{i,j}} + \sigma_{C_{i,j}} / \mathbf{K}_{xP})$		[C19i]

$$\delta M_{Bi,j} / \delta t = \Sigma_z [R_{gi,j} (1 - Y_{gi,z}) / Y_{gi,z}] - R_{si,j} - l_{i,j,C}$$

branch growth driven by R_g [C20a]

$$\delta M_{Ri,r,l} / \delta t = [R_{gi,r,l} (1 - Y_{gi,r}) / Y_{gi,r}] - R_{si,r,l} - l_{i,r,l,C}$$

root growth driven by R_g [C20b]

$$\delta A_{Li,j,k,l} / \delta t = \chi [M_{Li,j,k,l} / y_i] \delta M_{Li,j,k,l} / \delta t \min\{1, \max\{0, \psi_i - \psi_i'\}\}$$

leaf expansion driven by leaf mass [C21a]

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

growth
root extension of primary and [C21b]

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

secondary axes driven by root [C21c]

$$f_{tai} T_{ci} \{\exp[B_v - H_{av} / (RT_{ci})]\} / \{1 + \exp[(H_{di} - ST_{ci}) / (RT_{ci})] + \exp[(ST_{ci} - H_{dh}) / (RT_{ci})]\}$$

Arrhenius function for R_a [C22a]

$$f_{tmi} e^{(0.0811 (T_{ci} - 298.15))}$$

temperature function for R_m [C22b]

Root and Mycorrhizal Nutrient Uptake

$$U_{NH4i,r,l} = \{U_{wi,r,l} [NH_4^-] + 2\pi L_{i,r,l} D_{eNH4l} ([NH_4^-] - [NH_4^-]_{i,r,l}) / \ln(d_{i,r,l} / r_{ri,r,l})\}$$

root N and P uptake from mass [C23a]

$$= U'_{NH4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NH_4^-]_{i,r,l} - [NH_4^-]_{mn}) / ([NH_4^-]_{i,r,l} - [NH_4^-]_{mn} + K_{NH4}) f_{tai,l} f_{iNi,r,l}$$

flow + diffusion coupled with [C23b]

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

active uptake of NH_4^+ , NO_3^- and [C23c]

$$= U'_{NO3} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([NO_3^-]_{i,r,l} - [NO_3^-]_{mn}) / ([NO_3^-]_{i,r,l} - [NO_3^-]_{mn} + K_{NO3}) f_{tai,l} f_{iNi,r,l}$$

as modelled for microbial N and P [C23d]

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

[C23e]

$$= U'_{PO4} (U_{O2i,r,l} / U'_{O2i,r,l}) A_{i,r,l} ([H_2PO_4^-]_{i,r,l} - [H_2PO_4^-]_{mn}) / ([H_2PO_4^-]_{i,r,l} - [H_2PO_4^-]_{mn} + K_{PO4}) f_{tai,l} f_{iPi,r,l}$$

[C23f]

$$f_{iNi,r,l} = \sigma_{Ci,r,l} / (\sigma_{Ci,r,l} + \sigma_{Ni,r,l} / K_{iNC})$$

product inhibition of U_{NH4} , U_{NO3} [C23g]

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

and U_{PO4} determined by σ_N and σ_P [C23h]

vs. σ_C in roots

C₄ Gross Primary Productivity

C₄ Mesophyll

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

[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]
$r_{fi,j,k,l,m,n,o} = r_{fmini,j,k,l,m,n,o} + (r_{fmaxi} - r_{fmini,j,k,l,m,n,o}) e^{(-\beta \psi_i)}$		[C27]
$r_{fmini,j,k,l,m,n,o} = (C_b - C_{i(m4)}) / V_{c0(m4)ij,k,l,m,n,o}$		[C28]
$V_{b(m4)ij,k,l,m,n,o} = V_{bmax(m4)ij,k} (C_{c(m4)ij,k,l,m,n,o} - \Gamma_{(m4)ij,k}) / (C_{c(m4)ij,k,l,m,n,o} + K_{c(m4)i})$	CO ₂ -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	[C30a]
$Y_{(m4)ij,k} = (C_{c(m4)ij,k,l,m,n,o} - \Gamma_{(m4)ij,k}) / (3.0 C_{c(m4)ij,k,l,m,n,o} + 10.5 \Gamma_{(m4)ij,k})$		[C30b]
$J_{(m4)ij,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{max(m4)ij,k} - ((\varepsilon I_{i,l,m,n,o} + J_{max(m4)ij,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{max(m4)ij,k})^{0.5}) / (2\alpha)$	irradiance response function	[C31]
$V_{bmax(m4)ij,k} = V_{bmax(m4)}' [N_{pep(m4)ij,k}]' N_{fi,j,k} A_{fi,j,k} f_{C(m4)ij,k} f_{\psi_i} f_{tbi}$	PEPc activity	[C32]
$J_{max(m4)ij,k} = J_{max}' [N_{chl(m4)ij,k}]' N_{fi,j,k} A_{fi,j,k} f_{C(m4)ij,k}, f_{\psi_i} f_{tji}$	chlorophyll activity	[C33]
$f_{C(m4)ij,k} = 1.0 / (1.0 + [\chi_{C4(m4)ij,k}] / K_{\chi_{C4(m4)}})$	C ₄ product inhibition	[C34]
$f_{\psi_{ij,k,l,m,n,o}} = (r_{fmin_{ij,k,l,m,n,o}} / r_{fi,j,k,l,m,n,o})^{0.5}$	non-stomatal water limitation	[C35]

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]
$\delta \chi_{C4(m4)ij,k} / \delta t = \Sigma_{l,m,n,o} V_{c(m4)ij,k,l,m,n,o} - V_{\chi_{C4(m4)ij,k}}$	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]
$\delta C_{c(b4)ij,k} / \delta t = V_{\chi_{C4(b4)ij,k}} - V_{\phi(b4)ij,k} - \Sigma_{l,m,n,o} V_{c(b4)ij,k,l,m,n,o}$	bundle sheath CO ₂ 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]
$V_{b(b4)ij,k} = V_{\max(b4)ij,k} (C_{c(b4)ij,k} - \Gamma_{(b4)ij,k}) / (C_{c(b4)ij,k} + K_{c(b4)i})$	CO ₂ -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	[C45a]
$Y_{(b4)ij,k} = (C_{c(b4)ij,k} - \Gamma_{(b4)ij,k}) / (4.5 C_{c(b4)ij,k} + 10.5 \Gamma_{(b4)ij,k})$	carboxylation efficiency of $V_{j(b4)}$	[C45b]
$J_{(b4)ij,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\max(b4)ij,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\max(b4)ij,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\max(b4)ij,k})^{0.5}) / (2\alpha)$	irradiance response function	[C46]
$V_{\max(b4)ij,k} = V_{\max(b4)}' [N_{rub(b4)ij,k}]' N_{fii,j,k} A_{lfii,j,k} f_{C(c3)ij,k} f_{\psi i} f_{vi}$	RuBPC activity	[C47]
$J_{\max(b4)ij,k} = J_{\max}' [N_{chl(b4)ij,k}]' N_{fii,j,k} A_{lfii,j,k} f_{C(c3)ij,k} f_{\psi i} f_{vi}$	chlorophyll activity	[C48]
$f_{C(c3)ij,k} = \min\{[\nu_{fii,j}] / ([\nu_{lfii,j}] + [\chi_{c3(b4)ij}] / K_{I\nu_{lf}}), [\pi_{fii,j}] / ([\pi_{lfii,j}] + [\chi_{c3(b4)ij}] / K_{I\pi_{lf}})\}$	C ₃ product inhibition	[C49]

Shoot – Root - Mycorrhizal C, N, P Transfer

$Z_{sCi,j-i,r,l} = g_{sCi,j-i,r,l} (\sigma_{Ci,j} M_{Ri,r,l} - \sigma_{Ci,r,l} M_{Bi,j}) / (M_{Ri,r,l} + M_{Bi,j})$	shoot – root C transfer driven by σ_C concentration gradients	[C50]
$Z_{sN,Pi,j-i,r,l} = g_{sN,Pi,j-i,r,l} (\sigma_{N,Pi,j} \sigma_{Ci,r,l} - \sigma_{N,Pi,r,l} \sigma_{Ci,j}) / (\sigma_{Ci,r,l} + \sigma_{Ci,j})$	shoot – root N,P transfer driven by $\sigma_{N,P}$ concentration gradients	[C51]
$Z_{rCi,j-i,r,l} = g_{rCi,j-i,r,l} (\sigma_{Ci,r,l} M_{Mi,r,l} - \sigma_{Ci,m,l} M_{Ri,r,l}) / (M_{Mi,r,l} + M_{Ri,r,l})$	root – mycorrhizal C transfer driven by σ_C conc'n gradients	[C52]
$Z_{rN,Pi,j-i,r,l} = g_{rN,Pi,j-i,r,l} (\sigma_{N,Pi,r,l} \sigma_{Ci,m,l} - \sigma_{N,Pi,m,l} \sigma_{Ci,r,l}) / (\sigma_{Ci,m,l} + \sigma_{Ci,r,l})$	root – mycorrhizal N,P transfer driven by $\sigma_{N,P}$ conc'n gradients	[C53]

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				

l	soil or canopy layer
m	leaf azimuth
n	leaf inclination
o	leaf exposure (sunlit vs. shaded)
z	organ including leaf, stem, root r , mycorrhizae m

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_j	parameter such that $f_{tji} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10c]	17.354	
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]	24.212	
B_v	parameter such that $f_{tvi} = 1.0$ at $T_c = 298.15 \text{ K}$		[C10a, C22]	26.229	
C_b	$[\text{CO}_2]$ in canopy air	$\mu\text{mol mol}^{-1}$	[C2,C5 C25,C28]		
C_c	$[\text{CO}_2]$ in canopy chloroplasts in equilibrium with $C_{i,j,k,l,m,n,o}$	μM	[C6a,C7b]		
$C_{c(b4)}$	$[\text{CO}_2]$ in C_4 bundle sheath	μM	[C38,C39,C42,C4 4,C45b]		
$C_{c(m4)}$	$[\text{CO}_2]$ in C_4 mesophyll in equilibrium with $C_{i,j,k,l,m,n,o}$	μM	[C29,C30b,C39]		
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	$[\text{CO}_2]$ in canopy leaves	$\mu\text{mol mol}^{-1}$	[C2]		
$C_{i(m4)}'$	$[\text{CO}_2]$ in C_4 mesophyll air when $\psi_{ci} = 0$	$\mu\text{mol mol}^{-1}$	[C28]	$0.45 \times C_b$	

$C_{i(m4)}$	[CO ₂] in C ₄ mesophyll air	μmol mol ⁻¹	[C25]		
$C_{i,j,z=l}$	C content of leaf ($z = l$)	g C m ⁻²	[C18]		
$D_{e\text{ NH}_4l}$	effective dispersivity-diffusivity of NH ₄ ⁺ during root uptake	m ² h ⁻¹	[C23]		
$D_{e\text{ NO}_3l}$	effective dispersivity-diffusivity of NO ₃ ⁻ during root uptake	m ² h ⁻¹	[C23]		
$D_{e\text{ PO}_4l}$	effective dispersivity-diffusivity of H ₂ PO ₄ ⁻ during root uptake	m ² h ⁻¹	[C23]		
D_{rO2}	aqueous diffusivity of O ₂ from root aerenchyma to root or mycorrhizal surfaces	m ² h ⁻¹	[C14d]		
D_{sO2}	aqueous diffusivity of O ₂ from soil to root or mycorrhizal surfaces	m ² h ⁻¹	[C14d]		
$d_{i,r,l}$	half distance between adjacent roots assumed equal to uptake path length	m	[C23]	$(\pi L_{s,z} / \Delta z)^{-1/2}$	Grant (1998)
$E_{N,P}$	energy cost of nutrient uptake	g C g N ⁻¹ or P ⁻¹	[C13]	2.15	Veen (1981)
$f_{C(c3)} \square$	C ₃ product inhibition of RuBP carboxylation activity in C ₄ bundle sheath or C ₃ mesophyll	-□	[C47,C48,C49]		
$f_{C(m4)}$	C ₄ product inhibition of PEP carboxylation activity in C ₄ mesophyll	-□	[C32,C33,C34]		
F_{chl}	fraction of leaf protein in chlorophyll	-	[C8b]	0.025	
f_{iC}	N,P inhibition on carboxylation, leaf structural N,P growth	-	[C6a,C7,C11,C12]□ □		□
f_{iN}	N inhibition on root N uptake	-□	[C23g]	□	□
f_{iP}	P inhibition on root P uptake	-□	[C23h]	□	□
$f_{\lambda N}$	fraction of X_{mx} N translocated out of leaf or root before litterfall	-□	[C19a,c]	□	□
$f_{\lambda P}$	fraction of X_{mx} P translocated out of leaf or root before litterfall	-□	[C19b,d]	□	□

F_{rubisco}	fraction of leaf protein in rubisco	-	[C6b,d]	0.125	
f_{ta}	temperature effect on $R_{\text{ai},j}$ and U	—	[C14,C22,C23]□	□	□
f_{tb}	temperature effect on carboxylation	—	[C6b,C10a]□	□	□
f_{tj}	temperature effect on electron transport	□	[C8b,C10c]	□	□
f_{tke}	temperature effect on K_{c_i}	□	[C6e,C10d]	□	Bernacchi et al. (2001,2003)□
f_{tko}	temperature effect on K_{o_i}	□	[C6e,C10e]	□	Bernacchi et al. (2001,2003)□
f_{tm}	temperature effect on $R_{\text{mi},j}$	—	[C16, C22b]□	$Q_{\text{□□□□□□□□}}$	□
f_{to}	temperature effect on oxygenation	□	[C6d,C10b]		□
f_{tv}	temperature effect on carboxylation	—□	[C32,C33,C36,C47,C48]		
f_{xN}	inhibition of root or mycorrhizal N exudation	—□	[C19f,h]		
f_{xP}	inhibition of root or mycorrhizal P exudation	—□	[C19g,i]		
$f_{\psi i}$	non-stomatal water effect on carboxylation	—	[C6a,C7a,C9]□	□	Medrano et al. (2002)
$f_{\psi i}$	non-stomatal water effect on carboxylation	—□	[C32,C33,C35C47,C48]		
g_{sC}	conductance for shoot-root C transfer	h^{-1}	[C50]	calculated from root depth, axis number	Grant (1998)
$g_{\text{sN,P}}$	rate constant for shoot-root N,P transfer	h^{-1}	[C51]	0.1	Grant (1998)
g_{rC}	rate constant for root-mycorrhizal C transfer	h^{-1}	[C52]	0.1	Grant (1998)
$g_{\text{rN,P}}$	rate constant for root-mycorrhizal N,P transfer	h^{-1}	[C53]	0.1	Grant (1998)
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_{ci}	$J \text{ mol}^{-1}$	[C10d]	55×10^3	Bernacchi et al. (2001,2003) Bernacchi et al. (2001,2003) Bernacchi et al. (2001,2003) Bernacchi et al. (2001,2003)
H_{ako}	parameter for temperature sensitivity of K_{oi}	$J \text{ mol}^{-1}$	[C10e]	20×10^3	
H_{ao}	energy of activation for oxygenation	$J \text{ mol}^{-1}$	[C10b, C22]	60×10^3	
H_{av}	energy of activation for carboxylation	$J \text{ mol}^{-1}$	[C10a, C22]	65×10^3	
H_{dh}	energy of high temperature deactivation	$J \text{ mol}^{-1}$	[C10, C22]	222.5×10^3	
H_{dl}	energy of low temperature deactivation	$J \text{ mol}^{-1}$	[C10, C22]	197.5×10^3	Barber and Silberbush, 1984
$[H_2PO_4^-]_{i,r,l}$	concentration of $H_2PO_4^-$ root or mycorrhizal surfaces	$g \text{ N m}^{-3}$	[C23]		
$[H_2PO_4^-]_{mn}$	concentration of $H_2PO_4^-$ at root or mycorrhizal surfaces below which $U_{PO_4} = 0$	$g \text{ N m}^{-3}$	[C23]	0.002	
I	irradiance	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C8a,]		
J	electron transport rate in C ₃ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C7a,C8a]		
$J_{(b4)}$	electron transport rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C45a,C46]		Lawlor (1993)
$J_{(m4)}$	electron transport rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C30a,C31]		
J_{max}'	specific electron transport rate at non-limiting I and 25°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_{iC_N}	inhibition constant for growth in shoots from σ_C vs. σ_N	$g\ C\ g\ N^{-1}$	[C11]	100	Grant (1998)
K_{iC_P}	inhibition constant for growth in shoots from σ_C vs. σ_P	$g\ C\ g\ P^{-1}$	[C11]	1000	Grant (1998)
$K_{I/C4(b4)}$	constant for CO_2 product inhibition of C_4 decarboxylation in C_4 bundle sheath	μM	[C38]	1000.0	
$K_{I/C4(m4)}$	constant for C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	μM	[C34]	5×10^6	
K_{Ivlf}	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	
$K_{I\pi lf}$	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_{iN_C}	inhibition constant for N uptake in roots from σ_{Cij} vs. σ_{Nj}	$g\ N\ g\ C^{-1}$	[C23]	0.1	Grant (1998)
K_{iP_C}	inhibition constant for P uptake in roots from σ_{Cij} vs. σ_{Pij} roots	$g\ P\ g\ C^{-1}$	[C23]	0.01	Grant (1998)
$K_{\lambda N}$	inhibition constant for remobilization of leaf or root N during senescence	$g\ N\ g\ C^{-1}$	[C19c]	0.1	
$K_{\lambda P}$	inhibition constant for remobilization of leaf or root P during senescence	$g\ P\ g\ C^{-1}$	[C19d]	0.01	
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 $H_2PO_4^{-}$ 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]	0.32	Griffin (1972)

K_o	inhibition constant for O ₂ in carboxylation	$\square M$	[C6c,C6e]	500 at 25 °C	Farquhar et al. (1980)
K_{xN}	inhibition constant for exudation of root or mycorrhizal N	g C g N ⁻¹	[C19h]	1.0	
K_{xP}	inhibition constant for exudation of root or mycorrhizal P	g C g N ⁻¹	[C19i]	10.0	
L	root length	m m ⁻²	[C14d,C21b,C23]		
l_c	C litterfall from leaf or root	g C m ⁻² h ⁻¹	[C18,C19a,b,C20]		
$l_{N,P}$	N or P litterfall from leaf or root	g C m ⁻² h ⁻¹	[C19a,b]		
M_B	branch C phytomass	g C m ⁻²	[C20,C50]		
M_L	leaf C phytomass	g C m ⁻²	[C12,C21]		
M_{L_N}, M_{L_R}	non-remobilizable, remobilizable (protein) leaf C phytomass	g C m ⁻²	[C12,C18]		
M_M	mycorrhizal C phytomass	g C m ⁻²	[C52]		
M_R	root C phytomass	g C m ⁻²	[C20,C21,C50,C52]		
$M_{L_{iprot}}$	leaf protein phytomass calculated from leaf N, P contents	g N m ⁻²	[C6b,C6d,C8b]		
N,P	N or P content of organ z	g N m ⁻²	[C16, C19]		
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 x N_{leaf}	
N_{lr}	total leaf N	g N m ⁻² leaf	[C32,C33,C47,C48]		
N_{prot}	N content of protein remobilized from leaf or root	g N C ⁻¹	[C12,C19a]	0.4	
$[N_{chl(b4)}]'$	ratio of chlorophyll N in C ₄ bundle sheath to total leaf N	g N g N ⁻¹	[C48]	0.05	
$[N_{chl(m4)}]'$	ratio of chlorophyll N in C ₄ mesophyll to total leaf N	g N g N ⁻¹	[C33]	0.05	

$[\text{NH}_4^+_{i,r,l}]$	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
$[N_{\text{pep}(m4)}]'$	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	$[\text{O}_2]$ 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]	$0.33 \times P_{\text{leaf}}$	
P_{prot}	P content of protein remobilized from leaf or root	g P C^{-1}	[C12,C19b]	0.04	
$[\mathcal{M}_f]$	concentration of nonstructural root P uptake product in leaf	g P g C^{-1}	[C49]		
θ_p	root or mycorrhizal porosity	$\text{m}^3 \text{ m}^{-3}$	[C21b]	$0.1 - 0.5$	
R	gas constant	$\text{J mol}^{-1} \text{ K}^{-1}$	[C10, C22]	8.3143	
R_a	total autotrophic respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13]		
R_a'	R_a under nonlimiting O_2	$\text{g C m}^{-2} \text{ h}^{-1}$	[C14]		
R_c'	specific autotrophic respiration of $\sigma_{c,i,j}$ at $T_{ci} = 25^\circ\text{C}$	$\text{g C g C}^{-1} \text{ h}^{-1}$	[C14]	0.015	

R_c	autotrophic respiration of $\sigma_{Ci,j}$ or $\sigma_{Ci,r,l}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13,C14,C17, C15]		
R_g	growth respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C17,C20]		
r_{lf}	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 $T_{ci} = 25^\circ\text{C}$	$\text{g C g N}^{-1} \text{ h}^{-1}$	[C16]	0.0115	Barnes et al. (1998)
$R_{mi,j}$	above-ground maintenance respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[C16,C17,C15]		
$r_{qi,r,l}$	radius of root aerenchyma	m	[C14d]		
$r_{ri,r,l}$	root or mycorrhizal radius	m	[C14d,C21b,c,C23 a,c,e]	1.0×10^{-4} or 5.0×10^{-6}	
$R_{si,j}$	respiration from remobilization of leaf C	$\text{g C m}^{-2} \text{ h}^{-1}$	[C13,C15,C18, C20]		
r_{sl}	thickness of soil water films	m	[C14d]		
r_x	rate constant for root or mycorrhizal exudation	h^{-1}	[C19f,g,h]	0.001	
ρ_r	dry matter content of root biomass	g g^{-1}	[C21b]	0.125	
S	change in entropy	$\text{J mol}^{-1} \text{ K}^{-1}$	[C10, C22]	710	Sharpe and DeMichelle (1977)
σ_C	nonstructural C product of CO_2 fixation	g C g C^{-1}	[C11,C19c,d,e,h,i, C23g,h,C50-53]		

σ_N	nonstructural N product of root uptake	g N g C^{-1}	[C11, C19c,f,h,i C23g,h,C51,C53]		
σ_P	nonstructural P product of root uptake	g P g C^{-1}	[C11, C19d,g,h,i C23g,h,C51,C53]		
T_c	canopy temperature	K	[C10, C22]		
$U_{\text{NH}_4 i,r,l}$	NH_4^+ uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
U'_{NH_4}	maximum U_{NH_4} at 25 °C and non-limiting NH_4^+	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{\text{NO}_3 i,r,l}$	NO_3^- uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
U'_{NO_3}	maximum U_{NO_3} at 25 °C and non-limiting NO_3^-	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{\text{PO}_4 i,r,l}$	H_2PO_4^- uptake by roots or mycorrhizae	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]		
U'_{PO_4}	maximum U_{PO_4} at 25 °C and non-limiting H_2PO_4^-	$\text{g N m}^{-2} \text{ h}^{-1}$	[C23]	5.0×10^{-3}	Barber and Silberbush, 1984
$U_{\text{O}_2 i,r,l}$	O_2 uptake by roots and mycorrhizae under ambient O_2	$\text{g O m}^{-2} \text{ h}^{-1}$	[C14b,c,C23b,d,f]		
$U'_{\text{O}_2 i,l,r}$	O_2 uptake by roots and mycorrhizae under nonlimiting O_2	$\text{g O m}^{-2} \text{ h}^{-1}$	[C14b,c,C23b,d,f]		
$U_{\text{w},i,r,l}$	root water uptake	$\text{m}^3 \text{ m}^{-2} \text{ h}^{-1}$	[C14d,C23]		
$V_{\phi(\text{b4})i,j,k}$	CO_2 leakage from C_4 bundle sheath to C_4 mesophyll	$\text{g C m}^{-2} \text{ h}^{-1}$	[C39,C42]		
V_b'	specific rubisco carboxylation at 25 °C	$\mu\text{mol g}^{-1} \text{ rubisco}$ s^{-1}	[C6b]	45	Farquhar et al. (1980)
$V_{\text{b}(\text{b4})i,j,k}$	CO_2 -limited carboxylation rate in C_4 bundle sheath	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C43,C44]		
$V_{\text{b}(\text{m4})i,j,k,l,m,n,o}$	CO_2 -limited carboxylation rate in C_4 mesophyll	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C26]		
$V_{\text{bi},j,k,l,m,n,o}$	CO_2 -limited leaf carboxylation rate	$\mu\text{mol m}^{-2} \text{ s}^{-1}$	[C3,C6]		
$V_{\text{bmax}(\text{b4})}'$	RuBP carboxylase specific activity in C_4 bundle sheath at 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	$\mu\text{mol g}^{-1} \text{ s}^{-1}$	[C47]	75	

$V_{\text{bmax(b4)}}_{i,j,k}$	CO ₂ -nonlimited carboxylation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C44,C47]	150	
$V_{\text{bmax(m4)}}'$	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]		
$V_{\text{bmax(m4)}}_{i,j,k}$	CO ₂ -nonlimited carboxylation rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C29,C32]		
$V_{\text{bmaxi,j,k}}$	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]		
$V_{c(\text{b4})}_{i,j,k,l,m,n,o}$	CO ₂ fixation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C43]		
$V_{c(\text{m4})}_{i,j,k,l,m,n,o}$	CO ₂ fixation rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C24,C26,C40,C41]	450	Farquhar et al. (1980)
$V_{c0(\text{m4})}_{i,j,k,l,m,n,o}$	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]		
$V_g(\text{m4})_{i,j,k,l,m,n,o}$	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]	9.5	Farquhar et al. (1980)
V_j'	specific chlorophyll e^- transfer at 25 °C	$\mu\text{mol g}^{-1} \text{chlorophyll s}^{-1}$	[C8b]		
$V_j(\text{b4})_{i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C ₄ bundle sheath	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C43,C45a]		
$V_j(\text{m4})_{i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C ₄ mesophyll	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C26,C30a]		
$V_{ji,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	$\mu\text{mol m}^{-2} \text{s}^{-1}$	[C3,C7a]		
V_o'	specific rubisco oxygenation at 25 °C	$\mu\text{mol g}^{-1} \text{rubisco s}^{-1}$	[C6d]	9.5	Farquhar et al. (1980)
$V_{\text{omaxi,j,k}}$	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]		

$V_{\chi C4(m4)}$	transfer of C ₄ fixation product between C ₄ mesophyll and bundle sheath	$\text{g C m}^{-2} \text{ h}^{-1}$	[C37]		
$[v_f]$	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]		
$W_{lf(b4)}$	C ₄ bundle sheath water content	g m^{-2}	[C37,C39]		
$W_{lf(m4)}$	C ₄ mesophyll water content	g m^{-2}	[C37]		
X_{mx}	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	[C19a,b]	0.6	Kimmins (2004)
$x_{i,r,l,C}$	root and mycorrhizal C exudation	$\text{g C m}^{-2} \text{ h}^{-1}$	[C19e]		
$x_{i,r,l,N}$	root and mycorrhizal N exudation	$\text{g N m}^{-2} \text{ h}^{-1}$	[C19f]		
$x_{i,r,l,P}$	root and mycorrhizal P exudation	$\text{g P m}^{-2} \text{ h}^{-1}$	[C19g]		
Y	carboxylation yield from electron transport in C ₃ mesophyll	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C7a,b]		
$Y_{(b4)}$	carboxylation yield from electron transport in C ₄ bundle sheath	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C45a,b]		
$Y_{(m4)}$	carboxylation yield from electron transport in C ₄ mesophyll	$\mu\text{mol CO}_2 \mu\text{mol e}^{-1}$	[C30a,b]		
Y_g	fraction of σ_{Cij} used for growth expended as $R_{gij,z}$ by organ z	g C g C^{-1}	[C20]	0.28 (z = leaf), 0.24 (z = root and other non-foliar), 0.20 (z = wood)	Waring and Running (1998)
y	plant population	m^{-2}	[C21]		
Z_{sC}	shoot-root C transfer	$\text{g C m}^{-2} \text{ h}^{-1}$	[C50]		
$Z_{sN,P}$	shoot-root N,P transfer	$\text{g N,P m}^{-2} \text{ h}^{-1}$	[C51]		

Z_{rC}	root-mycorrhizal C transfer	$\text{g C m}^{-2} \text{ h}^{-1}$	[C52]		
$Z_{rN,P}$	root-mycorrhizal N,P transfer	$\text{g N,P m}^{-2} \text{ h}^{-1}$	[C53]		
Γ	CO ₂ compensation point in C ₃ mesophyll	μM	[C6a,C6c,C7b]		
$\Gamma_{(b4)}$	CO ₂ compensation point in C ₄ bundle sheath	μM	[C44,C45b]		
$\Gamma_{(m4)}$	CO ₂ compensation point in C ₄ mesophyll	μM	[C29,C30b]		
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	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[C8a]	0.45	Farquhar et al. (1980)
ε	quantum yield	$\mu\text{mol e}^{-} \mu\text{mol quanta}^{-1}$	[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_c	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]
$s_{x(x,y)} = 2 \text{ abs}[(Z + d_s + d_m)_{x,y} - (Z + d_s + d_m)_{x+1,y}] / (L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and pooled surface water in x (EW) and y (NS) directions	[D5b]
$s_{y(x,y)} = 2 \text{ abs}[(Z + d_s + d_m)_{x,y} - (Z + d_s + d_m)_{x,y+1}] / (L_{y(x,y)} + L_{y(x,y+1)})$		
$LE_l = L (e_a - e_l(T_l, \psi_l)) / r_{al}$	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

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

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

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

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

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

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

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

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

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

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

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

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

Exchange with Water Table

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

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

Heat Flux

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

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

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

y (NS) and z (vertical) directions

3D water transfer plus freeze-thaw [D8]

in direction x if source and [D9a]

destination cells are unsaturated
in direction x if source cell is [D9b]

saturated
in direction x if destination cell is

saturated [D9a]

in direction y if source and

destination cells are unsaturated
in direction y if source cell is [D9b]

saturated
in direction y if destination cell is

saturated [D9a]

in direction z if source and

destination cells are unsaturated
in direction z if source cell is [D9b]

saturated
in direction z if destination cell is

saturated

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

for each canopy, snow, residue and [D11]

soil surface, depending on exposure
3D conductive – convective heat [D12a]

flux among snowpack, surface
residue and soil layers in x (EW), y [D12b]

$$G_{z(x,y,z)} = 2 \kappa_{(x,y,z),(x,y,z+l)} (T_{(x,y,z)} - T_{(x,y,z+l)}) / (L_z(x,y,z) + L_z(x,y,z+l)) + c_w T_{(x,y,z)} Q_{wz(x,y,z)} \quad \text{(NS) and } z \text{ (vertical) directions} \quad [\text{D12c}]$$

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

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

Gas Flux

$$Q_{ds\gamma x,y,z} = a_{gsx,y,z} D_{d\gamma} (S'_{\gamma} f_{d_{\gamma x,y,z}} [\gamma_{gs}]_{x,y,z} - [\gamma_{ss}]_{x,y,z}) \quad \text{volatilization – dissolution between aqueous and gaseous phases in soil and root} \quad [\text{D14a}]$$

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

$$Q_{gs\gamma zx,y,l} = g_{ax,y} \{ [\gamma_a] - \{ 2 [\gamma_{gs}]_{x,y,l} D_{gs\gamma z(x,y,l)} / L_z(x,y,l) + g_{ax,y} [\gamma_a] \} / \{ 2 D_{gs\gamma z(x,y,l)} / L_z(x,y,l) + g_{ax,y} \} \} \quad \text{volatilization – dissolution between gaseous and aqueous phases at the soil surface } (z = l) \text{ and the atmosphere} \quad [\text{D15a}]$$

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

$$Q_{gs\gamma x(x,y,z)} = -Q_{wx(x,y,z)} [\gamma_{gs}]_{x,y,z} + 2 D_{gs\gamma x(x,y,z)} ([\gamma_{gs}]_{x,y,z} - [\gamma_{gs}]_{x+l,y,z}) / (L_x(x,y,z) + L_x(x+l,y,z)) \quad \text{3D convective - conductive gas flux among soil layers in } x \text{ (EW), } y \text{ (NS) and } z \text{ (vertical) directions,} \quad [\text{D16a}]$$

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

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

$$Q_{gr\gamma z(x,y,z)} = D_{gr\gamma z(x,y,z)} ([\gamma_{gr}]_{x,y,z} - [\gamma_a]) / \Sigma_{1,z} L_z(x,y,z) \quad \text{convective - conductive gas flux between roots and the atmosphere} \quad [\text{D16d}]$$

$$D_{gs\gamma x(x,y,z)} = D'_{g\gamma} f_{gx,y,z} [\theta_{gx,y,z} + \theta_{gx+l,y,z}]^2 / \theta_{psx,y,z}^{0.67} \quad \text{gasous diffusivity as a function of air-filled porosity in soil} \quad [\text{D17a}]$$

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

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

$$D_{gr\gamma z(x,y,z)} = D'_{g\gamma} f_{gx,y,z} [\theta_{prx,y,z}]^{1.33} A_r(x,y,z) / A_{x,y} \quad \text{gasous diffusivity as a function of air-filled porosity in roots} \quad [\text{D17d}]$$

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

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

Solute Flux

$$Q_{s\gamma x}(x,y,z) = -Q_{wx}(x,y,z) [\gamma_{ss}]_{x,y,z} + 2 D_{s\gamma x}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x+1,y,z}) / (L_x(x,y,z) + L_x(x+1,y,z))$$

3D convective - dispersive solute flux among soil layers in x (EW), y (NS) and z (vertical) directions [D19a]

$$Q_{s\gamma y}(x,y,z) = -Q_{wy}(x,y,z) [\gamma_{ss}]_{x,y,z} + 2 D_{s\gamma y}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y+1,z}) / (L_y(x,y,z) + L_y(x,y+1,z))$$

[D19b]

$$Q_{s\gamma z}(x,y,z) = -Q_{wz}(x,y,z) [\gamma_{ss}]_{x,y,z} + 2 D_{s\gamma z}(x,y,z) ([\gamma_s]_{x,y,z} - [\gamma_s]_{x,y,z+1}) / (L_z(x,y,z) + L_z(x,y,z+1))$$

[D19c]

$$Q_{r\gamma}(x,y,z) = -Q_{wr}(x,y,z) [\gamma_{ss}]_{x,y,z} + 2\pi [L_{i,r} D_{s\gamma}([\gamma_{ss}] - [\gamma_{tri,r}]) \ln\{(r_s / r_{ti,r}) / (r_{ti,r} / r_{ti,r})\} + 2\pi [L_{i,r} D_{r\gamma}([\gamma_{tri,r}] - [\gamma_{tri,r}]) \ln(r_{qi,r} / r_{ti,r})]$$

convective - dispersive solute flux between soil and root aqueous phases [D19d]

$$D_{s\gamma x}(x,y,z) = D_{qx}(x,y,z) |Q_{wx}(x,y,z)| + D'_{s\gamma} f_{sx,y,z} [\theta_{wx,y,z} + \theta_{wx+1,y,z}] \tau$$

aqueous dispersivity in soil as functions of water flux and water-filled porosity in x, y and z directions [D20a]

$$D_{s\gamma y}(x,y,z) = D_{qy}(x,y,z) |Q_{wy}(x,y,z)| + D'_{s\gamma} f_{sy,y,z} [\theta_{wy,y,z} + \theta_{wy+1,y,z}] \tau$$

[D20b]

$$D_{s\gamma z}(x,y,z) = D_{qz}(x,y,z) |Q_{wz}(x,y,z)| + D'_{s\gamma} f_{sz,y,z} [\theta_{wz,y,z} + \theta_{wz+1,y,z}] \tau$$

[D20c]

$$D_{r\gamma}(x,y,z) = D'_{qr} |Q_{wr}(x,y,z)| + D'_{s\gamma} f_{sx,y,z} \theta_{wx,y,z} \tau$$

aqueous dispersivity to roots as functions of water flux and water-filled porosity [D20d]

$$D_{qx}(x,y,z) = 0.5 \alpha (L_x(x,y,z) + L_x(x+1,y,z))^{\beta}$$

dispersivity as a function of water flow length [D21a]

$$D_{qy}(x,y,z) = 0.5 \alpha (L_y(x,y,z) + L_y(x,y+1,z))^{\beta}$$

[D21b]

$$D_{qz}(x,y,z) = 0.5 \alpha (L_z(x,y,z) + L_z(x,y,z+1))^{\beta}$$

[D21c]

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]	0.20	
β	dependence of D_q on L	-	[D21]	1.07	
c	heat capacity of soil	$MJ m^{-2} ^\circ C^{-1}$	[D13]		
c_w	heat capacity of water	$MJ m^{-3} ^\circ C^{-1}$	[D12]	4.19	
$D_{d\gamma}$	volatilization - dissolution transfer coefficient for gas 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,D 17a,b,c]		Millington and Quirk (1960)
$D'_{g\gamma}$	diffusivity of gas γ in air at $0^\circ C$	$m^2 h^{-1}$	[D17]	6.43×10^{-2} for $\gamma =$ O_2	Campbell (1985)

D'_{qr}	dispersivity in roots	m	[D20d]	0.004	
D_q	dispersivity in soil	m	[D20,D21]		
$D_{r\gamma}$	aqueous diffusivity of gas or solute γ in roots	$m^2 h^{-1}$	[D19d,D20d]		
$D_{s\gamma}$	aqueous diffusivity of gas or solute γ in soil	$m^2 h^{-1}$	[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	$g m^{-3}$	[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]		
$f_{d,\gamma}$	temperature dependence of S'_{γ}	-	[D14,D15b,D18]		Wilhelm et al. (1977)
f_g	temperature dependence of $D'_{g\gamma}$	-	[D17]		Campbell (1985)
f_s	temperature dependence of $D'_{s\gamma}$	-	[D20]		Campbell (1985)
G	soil surface heat flux	$m^3 m^{-2} h^{-1}$	[D11]		

G_x, G_y, G_z	soil heat flux in x, y or z directions	$\text{MJ m}^{-2} \text{ h}^{-1}$	[D12,D13]	
g_a	boundary layer conductance	m h^{-1}	[D15a]	
γ	gas (H_2O , CO_2 , O_2 , CH_4 , NH_3 , N_2O , N_2 , 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, D19d]	
$[\gamma_{tr}]$	aqueous concentration of gas γ at root surface	g m^{-3}	[D19b]	
$[\gamma_{ss}]$	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	$\text{MJ m}^{-1} \text{ h}^{-1} \text{ }^\circ\text{C}^{-1}$	[D12]	de Vries (1963)
L_i	root length	m m^{-2}	[D19d]	
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_l	latent heat flux from surface litter	[D6a]	$\text{MJ m}^{-2} \text{ h}^{-1}$	
LE_s	latent heat flux from soil surface	[D6b]	$\text{MJ m}^{-2} \text{ h}^{-1}$	

L	latent heat of evaporation	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]		
$Q_{\text{b}\gamma\text{z}}$	bubbling flux	$\text{g m}^{-2} \text{h}^{-1}$	[D18]		
$Q_{\text{dr}\gamma}$	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 in soil	$\text{g m}^{-2} \text{h}^{-1}$	[D19a,b,c]		
Q_{ry}	aqueous flux of gas or solute γ from soil and root aqueous phases to root surface	$\text{g m}^{-2} \text{h}^{-1}$	[D19d]		
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_{wr}	root water uptake	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D19d, D20d]		
$Q_{\text{wx}}, Q_{\text{wy}}, Q_{\text{wz}}$	subsurface water flow in x, y or z directions	$\text{m}^3 \text{m}^{-2} \text{h}^{-1}$	[D4,D7,D8,D12,D16,D19,D20]		
θ_g	air-filled porosity	$\text{m}^3 \text{m}^{-3}$	[D17a,b,c]		
θ_{pr}	root porosity	$\text{m}^3 \text{m}^{-3}$	[D17d]	dryland spp. 0.10 wetland spp. 0.20	Luxmoore et al. (1970a,b)
θ_{ps}	soil porosity	$\text{m}^3 \text{m}^{-3}$	[D17a,b,c]		
θ_w	water-filled porosity	$\text{m}^3 \text{m}^{-3}$	[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]		
$r_{qi,r}$	radius of root or mycorrhizal aerenchyma	m	[D19d]		
$r_{ri,r}$	root or mycorrhizal radius	m	[D19d]	1.0×10^{-4} or 5.0×10^{-6}	
r_s	thickness of soil water films	m	[D19d, D21d]		
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

$\text{Al}(\text{OH})_{3(s)} \Leftrightarrow (\text{Al}^{3+}) + 3 (\text{OH}^-)$	(amorphous $\text{Al}(\text{OH})_3$)	-33.0	[E1] ¹
$\text{Fe}(\text{OH})_{3(s)} \Leftrightarrow (\text{Fe}^{3+}) + 3 (\text{OH}^-)$	(soil Fe)	-39.3	[E2]
$\text{CaCO}_{3(s)} \Leftrightarrow (\text{Ca}^{2+}) + (\text{CO}_3^{2-})$	(calcite)	-9.28	[E3]
$\text{CaSO}_{4(s)} \Leftrightarrow (\text{Ca}^{2+}) + (\text{SO}_4^{2-})$	(gypsum)	-4.64	[E4]
$\text{AlPO}_{4(s)} \Leftrightarrow (\text{Al}^{3+}) + (\text{PO}_4^{3-})$	(variscite)	-22.1	[E5] ²
$\text{FePO}_{4(s)} \Leftrightarrow (\text{Fe}^{3+}) + (\text{PO}_4^{3-})$	(strengite)	-26.4	[E6]
$\text{Ca}(\text{H}_2\text{PO}_4)_{2(s)} \Leftrightarrow (\text{Ca}^{2+}) + 2 (\text{H}_2\text{PO}_4^-)$	(monocalcium phosphate)	-1.15	[E7] ³
$\text{CaHPO}_{4(s)} \Leftrightarrow (\text{Ca}^{2+}) + (\text{HPO}_4^{2-})$	(monetite)	-6.92	[E8]
$\text{Ca}_5(\text{PO}_4)_3\text{OH}_{(s)} \Leftrightarrow 5 (\text{Ca}^{2+}) + 3 (\text{PO}_4^{3-}) + (\text{OH}^-)$	(hydroxyapatite)	-58.2	[E9]

*Cation Exchange Equilibria*⁴

$\text{X-Ca} + 2 (\text{NH}_4^+) \Leftrightarrow 2 \text{X-NH}_4 + (\text{Ca}^{2+})$	1.00	[E10]
$3 \text{X-Ca} + 2 (\text{Al}^{3+}) \Leftrightarrow 2 \text{X-Al} + 3 (\text{Ca}^{2+})$	1.00	[E11]
$\text{X-Ca} + (\text{Mg}^{2+}) \Leftrightarrow \text{X-Mg} + (\text{Ca}^{2+})$	0.60	[E12]
$\text{X-Ca} + 2 (\text{Na}^+) \Leftrightarrow 2 \text{X-Na} + (\text{Ca}^{2+})$	0.16	[E13]
$\text{X-Ca} + 2 (\text{K}^+) \Leftrightarrow 2 \text{X-K} + (\text{Ca}^{2+})$	3.00	[E14]
$\text{X-Ca} + 2 (\text{H}^+) \Leftrightarrow 2 \text{X-H} + (\text{Ca}^{2+})$	1.00	[E15]

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).

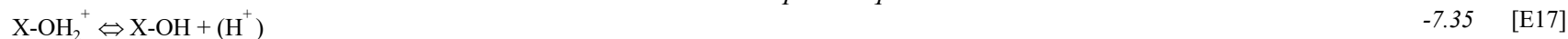
² All equilibrium reactions involving N and P are calculated for both band and non-band volumes if a banded fertilizer application has been made. These volumes are calculated dynamically from diffusive transport of soluble N and P.

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.

$$3 \text{ X-Al} + 2 (\text{X-Ca} + \text{X-Mg}) + \text{X-NH}_4 + \text{X-K} + \text{X-Na} + \text{X-H} = \text{CEC} \quad [\text{E16}]$$

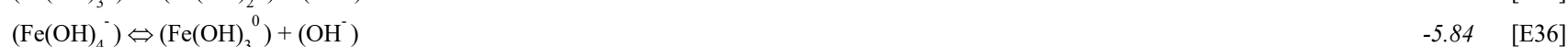
Anion Adsorption Equilibria



Organic Acid Equilibria



Ion Pair Equilibria



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

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]
$f_t = T_l \{ \exp[B - H_a / (R T_l)] \} / \{ 1 + \exp[(H_{dl} - ST_l) / (RT_l)] + \exp[(ST_l - H_{dh}) / (R T_l)] \}$	Arrhenius function	[F2]
$f_{NP} = \min \{ [N_{ni,l}] / [N_n'], [P_{ni,l}] / [P_n'] \}$	N or P limitation	[F3]
$R_{i,l} = R_{\max i,l} (V_{O_2 i,l} / V_{O_2 \max i,l})$	O ₂ limitation	[F4]
$V_{O_2 \max i,l} = 2.67 R_{\max i,l}$	O ₂ demand	[F5]
$V_{O_2 i,l} = V_{O_2 \max i,l} [O_{2ri,l}] / ([O_{2ri,l}] + K_{O_2 r})$	equilibrate O ₂ uptake with	[F6a]
$= 2\pi L_{ri,l} D_{sO_2} ([O_{2l}] - [O_{2ri,l}]) / \ln((r_{ri,l} + r_{wl}) / r_{ri,l})$	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]
$LC_{i,l} = R_{si,l} \min \{ M_{ni,l} / (2.5 N_{ni,l}), M_{ni,l} / (25.0 P_{ni,l}) \}$	microbial C litterfall	[F11]

N₂ Fixation

$V_{N_2 i,l} = \min \{ R_{gi,l} E_{N_2}' f_{CP}, M_{ni,l} [N_n'] - [N_{ni,l}] [N_{2ri,l}] / ([N_{2ri,l}] + K_{N_2 r}) \}$	rate of N ₂ fixation	[F12]
$f_{CP} = \min \{ [\chi_{ni,l}] / (1.0 + [\nu_{ni,l}] / K_{I\chi n}), [\pi_{ni,l}] / (1.0 + [\nu_{ni,l}] / K_{I\pi n}) \}$	product inhibition of N ₂ fixation	[F13]
$R_{N_2 i,l} = V_{N_2 i,l} / E_{N_2}'$	fixation respiration	[F14]
$U_{\chi i,l} = (R_{gi,l} - R_{N_2 i,l}) / (1 - Y_n')$	growth respiration	[F15]

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

Nodule – Root Exchange

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

Definition of Variables in Appendix F

Variable	Definition	Units	Equations	Input Values	Reference
B	parameter such that $f_i = 1.0$ at $T_i = 298.15$ 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_{LCI}	fraction of nodule C litterfall remobilized as nonstructural C	-	F24		
F_{LNI}	fraction of nodule N litterfall remobilized as nonstructural N	-	F25		
F_{LPI}	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_{χ^n}	Michaelis-Menten constant for nodule respiration of $\chi_{ndi,l}$	g g^{-1}	F1	0.01	
$K_{I\chi_n}$	inhibition constant for nonstructural N:C on N_2 fixation	g g^{-1}	F13	10	
$K_{I\pi_n}$	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	0.32
κ	rate constant for nonstructural C,N,P exchange between root and nodule	h^{-1}	F21,F22,F23	
$L_{ri,l}$	root length	$m\ m^{-2}$	F6b	
$L_{Ci,l}$	nodule C litterfall	$g\ C\ m^{-2}\ h^{-1}$	F11,F16,F24	
$L_{Ni,l}$	nodule N litterfall	$g\ N\ m^{-2}\ h^{-1}$	F19,F25	
$L_{Pi,l}$	nodule P litterfall	$g\ P\ m^{-2}\ h^{-1}$	F20,F26	
$M_{ni,l}$	nodule structural C	$g\ C\ m^{-2}$	F1,F11,F12,F16 ,F17,F18,F21	
$M_{ri,l}$	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	$\text{g C m}^{-2} \text{h}^{-1}$	F4,F9,F10,F24	
R_m	specific nodule maintenance respiration at 25°C	$\text{g C g C}^{-1} \text{h}^{-1}$	F7	
$R_{maxi,l}$	nodule respiration under non-limiting O ₂	$\text{g C m}^{-2} \text{h}^{-1}$	F1,F4,F5	
$R_{mi,l}$	nodule maintenance respiration	$\text{g C m}^{-2} \text{h}^{-1}$	F7,F9,F10,F24	
$R_{N_2i,l}$	nodule respiration for N ₂ fixation	$\text{g C m}^{-2} \text{h}^{-1}$	F14,F15,F24	
$R_{si,l}$	nodule senescence respiration	$\text{g C m}^{-2} \text{h}^{-1}$	F9,F11	
$r_{ri,l}$	root radius	m	F6b	
r_{wl}	radius of soil water films	m	F6b	
S	change in entropy	$\text{J mol}^{-1} \text{K}^{-1}$	F2	710
T_l	soil temperature	K	F2,F8	

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

Appendix G: CH₄ Production and Consumption

Anaerobic Fermenters and H₂ Producing Acetogens

$R_{i,f} = \{ \mathbf{R}'_f M_{i,f,a} [Q_{i,c}] / (\mathbf{K}_f (1 + [O_2] / \mathbf{K}_i) + [Q_{i,c}]) \} f_t$	respiration by fermenters		[G1]
$Q_{i,c} \rightarrow 0.67 A_{i,c} + 0.33 \text{ CO}_2\text{-C} + 0.11 \text{ H}_2$	partition respiration products		[G2]
$U_{i,f,c} = R_{m,i,f} + (R_{i,f} - R_{m,i,f}) (1.0 + Y_f)$	uptake of DOC by fermenters	$[R_{i,f} > R_{m,i,f}]$	[G3a]
$U_{i,f,c} = R_{i,f}$		$[R_{i,f} < R_{m,i,f}]$	[G3b]
$Y_f = -\Delta G_f / E_M$	growth yield of fermentation		[G4]
$\Delta G_f = \Delta \mathbf{G}'_f + \{ \mathbf{R} T \ln([H_2] / [H_2']^4) \}$	free energy change of fermentation		[G5]
$\delta M_{i,f,j,c} / \delta t = F_j U_{i,f,c} - F_j R_{i,f} - D_{i,f,j,c}$	growth of fermenters	$[R_{i,f} > R_{m,i,f}]$	[G6a]
$\delta M_{i,f,j,c} / \delta t = F_j U_{i,f,c} - R_{m,i,f,j} - D_{i,f,j,c}$		$[R_{i,f} < R_{m,i,f}]$	[G6b]

Acetotrophic Methanogens

$R_{i,m} = \{ \mathbf{R}'_m M_{i,m,a} [A_{i,c}] / (\mathbf{K}_m + [A_{i,c}]) \} f_t$	respiration by acetotrophic methanogens		[G7]
$A_{i,c} \rightarrow 0.50 \text{ CH}_4\text{-C} + 0.50 \text{ CO}_2\text{-C}$	partition respiration products		[G8]
$U_{i,m,c} = R_{m,i,m} + (R_{i,m} - R_{m,i,m}) (1.0 + Y_m)$	uptake by acetotrophic methanogens	$[R_{i,m} > R_{m,i,m}]$	[G9a]
$U_{i,m,c} = R_{i,m}$		$[R_{i,m} < R_{m,i,m}]$	[G9b]
$-Y_m = -\Delta \mathbf{G}'_m / E_M$	growth yield of acetotrophic methanogenesis		[G10]
$\delta M_{i,m,j,c} / \delta t = F_j U_{i,m,c} - F_j R_{i,m} - D_{i,m,j,c}$	growth of acetotrophic methanogens	$[R_{i,m} > R_{m,i,m}]$	[G11a]

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

Hydrogenotrophic Methanogens

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

Autotrophic Methanotrophs

$X'_t = \{ \mathbf{X}'_t M_{t,a} [CH_4] / (\mathbf{K}_t + [CH_4]) \} f_t \quad \square$	CH ₄ oxidation by methanotrophs under non-limiting O ₂	[G18]
$R'_t = X'_t Y_{tR}$	respiration by methanotrophs under non-limiting O ₂	[G19]
$Y_{tR} = -\Delta \mathbf{G}'_t / E_G$	energy yield from CH ₄ oxidation	[G20]
$X_t = X'_t f_{O_2t}$	CH ₄ oxidation by methanotrophs under ambient O ₂	[G21a]
$R_t = R'_t f_{O_2t}$	respiration by methanotrophs under ambient O ₂	[G21b]
$CH_4-C + 4.0 O_2 \rightarrow CO_2-C + 1.5 H_2O + 0.167 H^+$	O ₂ requirements for CH ₄ oxidation by methanotrophs	[G22]
$CH_4-C + 1.33 O_2 \rightarrow CH_2O-C + 0.167 H^+$	O ₂ requirements for growth by methanotrophs	[G23]

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

Definition of Variables in Appendix G

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

E_G	energy required to transform CH ₄ into organic C	kJ g C ⁻¹	[G20]	23.5	Anthony (1982)
E_M	energy required to construct new M from organic C	kJ g C ⁻¹	[G4,G10,G26]	25	
F_j	partitioning coefficient for j in $M_{i,n,j}$		[G6,G11,G17,G27]		
f	descriptor for fermenters and acetogens in each M_i				
f_{O_2t}	ratio of O ₂ uptake to O ₂ requirement for CH ₄ oxidation		[G21a,b]		
f_t	temperature function for growth-related processes (dimensionless)		[G1,G7,G12]		
$\Delta G'_c$	free energy change of C oxidation-O ₂ reduction	kJ g C ⁻¹	[G26]	-37.5	Brock and Madigan (1991)
ΔG_f	free energy change of fermentation plus acetogenesis	kJ g $Q_{i,c}^{-1}$	[G4,G5]		
$\Delta G'_f$	ΔG_f when $[H_2] = [H_2']$	kJ g $Q_{i,c}^{-1}$	[G5]	-4.43	Brock and Madigan (1991), Schink (1997)
ΔG_h	free energy change of hydrogenotrophic methanogenesis	kJ g CO ₂ -C ⁻¹	[G15,G16]		
$\Delta G'_h$	free energy change of hydrogenotrophic methanogenesis when $[H_2] = [H_2']$	kJ g CO ₂ -C ⁻¹	[G16]	-0.27	Brock and Madigan (1991)
$\Delta G'_m$	free energy change of acetotrophic methanogenesis	kJ g $A_{i,c}^{-1}$	[G10]	-1.03	
$\Delta G'_t$	free energy change of CH ₄ oxidation by methanotrophs	kJ g CH ₄ -C ⁻¹	[G20]	-9.45	Brock and Madigan (1991)

[H ₂]	aqueous concentration of H ₂	g H m ⁻³	[G5,G12,G16]		
[H ₂ ']	aqueous concentration of H ₂ when $\Delta G_h = \Delta G'_h$ and $\Delta G_f = \Delta G'_f$	g H m ⁻³	[G5,G16]	2.0 x 10 ⁻⁴	Brock and Madigan (1991)
<i>h</i>	descriptor for hydrogenotrophic methanogens in each M _{<i>i</i>}				
<i>i</i>	descriptor for organic matter-microbe complex (<i>i</i> = plant residue, manure, particulate OM, or humus)				
<i>j</i>	descriptor for structural or kinetic components for each functional type within each M _{<i>i</i>} (<i>e.g.</i> <i>a</i> = <i>active</i>)				
K_c	M-M constant for uptake of CO ₂ by hydrogenotrophic methanogens	g C m ⁻³	[G12]	0.12	
K_f	M-M constant for uptake of DOC _{<i>i,c</i>} by fermenters and acetogens	g C m ⁻³	[G1]	12	McGill et al. (1981)
K_i	inhibition constant for O ₂ on fermentation	g O m ⁻³	[G1]	0.32	
K_h	M-M constant for uptake of H ₂ by hydrogenotrophic methanogens	g H m ⁻³	[G12]	0.01	Mosey (1983), Robinson and Tiedje (1982)
K_m	M-M constant for uptake of A _{<i>i,c</i>} by acetotrophic methanogens	g C m ⁻³	[G7]	12	Smith and Mah (1978), Zehnder et al. (1980)
K_t	M-M constant for uptake of CH ₄ by methanotrophs	g C m ⁻³	[G18]	3 x 10 ⁻³	Conrad (1984)
<i>k</i>	descriptor for elemental fraction within each <i>j</i> (<i>j</i> = <i>c</i> , <i>n</i> or <i>p</i>)				
M	microbial communities	g C m ⁻²			
M _{<i>h</i>}	hydrogenotrophic methanogen community	g C m ⁻²	[G12,G17]		
M _{<i>i,f</i>}	fermenter and acetogenic community	g C m ⁻²	[G1,G6]		

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

$R_{m,t,j}$	maintenance respiration by methanotrophs	$\text{g C m}^{-2} \text{ h}^{-1}$	[G25,G27]		
R_t	CH ₄ oxidation by methanotrophs for respiration	$\text{g C m}^{-2} \text{ h}^{-1}$	[G21b,G23,G24, G25,G27a]		
R'_t	CH ₄ oxidation by methanotrophs for respiration at saturating O ₂	$\text{g C m}^{-2} \text{ h}^{-1}$	[G19,G21b]		
T	soil temperature	K	[G5,G16]		
t	descriptor for autotrophic methanotrophs				
$U_{h,c}$	rate of CO ₂ uptake by M_h	$\text{g C m}^{-2} \text{ h}^{-1}$	[G14,G17,G18]		
$U_{i,f,k}$	rate of DOC _{i,k} uptake by $M_{i,f}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G3,G6]		
$U_{i,m,c}$	rate of A _{i,c} uptake by $M_{i,m}$	$\text{g C m}^{-2} \text{ h}^{-1}$	[G9,G11]		
$U_{t,c}$	rate of CH ₄ uptake by M_t	$\text{g C m}^{-2} \text{ h}^{-1}$	[G25,G27]		
X_t	CH ₄ oxidation by methanotrophs	$\text{g C m}^{-2} \text{ h}^{-1}$	[G21a,G22]		
X'_t	CH ₄ oxidation by methanotrophs at saturating O ₂	$\text{g C m}^{-2} \text{ h}^{-1}$	[G1,G2,G4a]		
X'_t	specific CH ₄ oxidation by methanotrophs at saturating O ₂ , 30 °C and zero water potential	$\text{g C g}^{-1} \text{ h}^{-1}$	[G18]	0.5	Conrad (1984)
Y_f	biomass yield from fermentation and acetogenic reactions	$\text{g } M_{i,f} \text{ g } Q_{i,c}^{-1}$	[G3,G4]		
Y_h	biomass yield from hydrogenotrophic methanogenic reaction	$\text{g } M_h \text{ g CO}_2\text{-C}^{-1}$	[G14,G15,G18]		
Y_m	biomass yield from acetotrophic methanogenic reaction	$\text{g } M_{i,m} \text{ g } A_{i,c}^{-1}$	[G9,G10]		
Y_{tG}	biomass yield from methanotrophic growth respiration	$\text{g } M_t\text{-C g CH}_4\text{-C}^{-1}$	[G25a,G26]		
Y_{tR}	ratio of CH ₄ respired vs. CH ₄ oxidized by methanotrophs	g C g C^{-1}	[G19,G20]		

Appendix H: Inorganic N Transformations

Mineralization and Immobilization of Ammonium by All Microbial Populations

$$I_{NH_4i,n,j} = (M_{i,m,j,C} C_{Nj} - M_{i,m,j,N}) \quad (I_{NH_4i,n,j} < 0) \quad [H1a]$$

$$I_{NH_4i,n,j} = (M_{i,m,j,C} C_{Nj} - M_{i,m,j,N}) [NH_4^+] / ([NH_4^+] + K_{NH_4m}) \quad (I_{NH_4i,n,j} > 0) \quad [H1b]$$

$$I_{NO_3i,n,j} = (M_{i,m,j,C} C_{Nj} - (M_{i,m,j,N} + I_{NH_4i,n,j})) [NO_3^-] / ([NO_3^-] + K_{NO_3m}) \quad (I_{NO_3i,n,j} > 0) \quad [H1b]$$

Oxidation of DOC and Reduction of Oxygen by Heterotrophs

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

$$R'_{O_{2i,h}} = R_{QC} X'_{DOCi,h} \quad [H3]$$

$$R_{O_{2i,h}} = 4\pi\bar{n} M_{i,h,a} D_{SO_2} ([O_{2s}] - [O_{2mi,h}]) [r_m r_w / (r_w - r_m)] \quad [H4a]$$

$$= R'_{O_{2i,h}} [O_{2mi,h}] / ([O_{2mi,h}] + K_{O_2h}) \quad [H4b]$$

$$X_{DOCi,h} = X'_{DOCi,h} R_{O_{2i,h}} / R'_{O_{2i,h}} \quad [H5]$$

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

$$R'_{NO_3i,d} = E_{No_x} f_e (R'_{O_{2i,d}} - R_{O_{2i,d}}) \quad [H6]$$

$$R_{NO_3i,d} = R'_{NO_3i,d} [NO_3^-] / ([NO_3^-] + K_{NO_3d}) \quad [H7]$$

$$R_{NO_2i,d} = (R'_{NO_3i,d} - R_{NO_3i,d}) [NO_2^-] / ([NO_2^-] + K_{NO_2d}) \quad [H8]$$

$$R_{N_2Oi,d} = 2 (R'_{NO_3i,d} - R_{NO_3i,d} - R_{NO_2i,d}) [N_2O] / ([N_2O] + K_{N_2Od}) \quad [H9]$$

$$X_{DOCi,d} = X_{DOCi,d} (\text{from [H5]}) + F_{No_x} (R_{NO_3i,d} + R_{NO_2i,d}) + F_{N_2O} R_{N_2Oi,d} \quad [H10]$$

Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers

$$X'_{NH_3i,n} = X'_{NH_3} M_{i,n,a} \{[NH_3S] / ([NH_3S] + K_{NH_3n})\} \{[CO_2S] / ([CO_2S] + K_{CO_2})\} f_t \quad [H11]$$

$$R'_{O_{2i,n}} = R_{QN_3} X'_{NH_3i,n} + R_{QC} X'_{Ci,n} \quad [H12]$$

$$R_{O_{2i,n}} = 4\pi\bar{n} M_{i,n,a} D_{SO_2} (r_m r_w / (r_w - r_m)) ([O_{2s}] - [O_{2mi,n}]) \quad [H13a]$$

$$= R'_{O_{2i,n}} [O_{2mi,n}] / ([O_{2mi,n}] + K_{O_2n}) \quad [H13b]$$

$$X_{NH_3i,n} = X'_{NH_3i,n} R_{O_{2i,n}} / R'_{O_{2i,n}} \quad [H14]$$

Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers

$$X'_{NO_2i,o} = X'_{NO_2} M_{i,o,a} \{[NO_2^-] / ([NO_2^-] + K_{NO_2o})\} \{[CO_2S] / ([CO_2S] + K_{CO_2})\} f_t \quad [H15]$$

$$R'_{O_{2i,o}} = R_{QNO_2} X'_{NO_2i,o} + R_{QC} X'_{Ci,o} \quad [H16]$$

$$\begin{aligned}
R_{O_2i,o} &= 4\pi n M_{i,o,a} D_{sO_2} (r_m r_w / (r_w - r_m)) ([O_{2s}] - [O_{2mi,o}]) & [H17a] \\
&= R'_{O_2i,o} [O_{2mi,o}] / ([O_{2mi,o}] + K_{O_2o}) & [H17b] \\
X_{NO_2i,o} &= X'_{NO_2i,o} R_{O_2i,o} / R'_{O_2i,o} & [H18]
\end{aligned}$$

Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers

$$\begin{aligned}
R_{NO_2i,n} &= E_{NO_x} f_e (R'_{O_2i,n} - R_{O_2i,n}) & [H19] \\
R_{NO_2i,n} &= R'_{NO_2i,n} \{ [NO_2^-] / ([NO_2^-] + K_{NO_2n}) \} \{ [CO_{2s}] / ([CO_{2s}] + K_{CO_2}) \} & [H20] \\
X_{NH_3i,n} &= X_{NH_3i,n} \text{ (from [H14])} + 0.33 R_{NO_2i,n} & [H21]
\end{aligned}$$

Definition of Variables in Appendix H

Name	Definition	Units	Equations	Input Values	Reference
<i>Subscripts</i>					
<i>a</i>	active component of $M_{i,m}$				
<i>d</i>	heterotrophic denitrifier population (subset of <i>h</i>)				
<i>h</i>	heterotrophic community (subset of <i>m</i>)				
<i>i</i>	substrate-microbe complex				
<i>j</i>	kinetic components of $M_{i,m}$				
<i>m</i>	all microbial communities				
<i>n</i>	autotrophic ammonia oxidizer population (subset of <i>m</i>)				
<i>o</i>	autotrophic nitrite oxidizer population (subset of <i>m</i>)				
<i>Variables</i>					
C_{Nj}	maximum ratio of $M_{i,m,j,N}$ to $M_{i,m,j,C}$ maintained by $M_{i,m,j}$	g N g C ⁻¹	[H1]	0.22 and 0.13 for <i>j</i> = labile and resistant	
[CO _{2s}]	CO ₂ concentration in soil solution	g C m ⁻³	[H11,H15,H20]		
[DOC _i]	concentration of dissolved decomposition products	g C m ⁻³	[H2]		
D_{sO_2}	aqueous dispersivity-diffusivity of O ₂	m ² h ⁻¹	[H4,H13,H17]		
E_{NO_x}	e ⁻ accepted by NO _x vs. O ₂ when oxidizing DOC	g N g O ₂ ⁻¹	[H6,H19]	28/32 = 0.875	

F_{NO_x}	e ⁻ donated by C vs. e ⁻ accepted by NO _x when oxidizing DOC	g C g N ⁻¹	[H10]	12/28 = 0.43	
F_{N_2O}	e ⁻ donated by C vs. e ⁻ accepted by N ₂ O when oxidizing DOC	g C g N ⁻¹	[H10]	6/28 = 0.215	
f_e	fraction of electrons not accepted by O ₂ transferred to N oxides	-	[H6,H19]	0.25	Koike and Hattori (1975)
f_t	temperature function for microbial processes	-	[H2,H11]		
$I_{NH_4i,n,j}$	mineralization ($I_{NH_4i,n,j} < 0$) or immobilization ($I_{NH_4i,n,j} > 0$) of NH ₄ ⁺ by $M_{i,n,j,C}$	g N m ⁻² h ⁻¹	[H1]		
$I_{NO_3i,n,j}$	immobilization ($I_{NO_3i,n,j} > 0$) of NO ₃ ⁻ by $M_{i,n,j,C}$	g N m ⁻² h ⁻¹	[H1]		
K_{CO_2}	Michaelis-Menten constant for reduction of CO _{2s} by $M_{i,n,a}$ and $M_{i,o,a}$	g C m ⁻³	[H11,H15,H20]	0.15	
K_{NH_3n}	M-M constant for oxidation of NH _{3s} by nitrifiers	g N m ⁻³	[H11]	0.01	Suzuki et al. (1974)
K_{NH_4m}	M-M constant for microbial NH ₄ ⁺ uptake	g N m ⁻³	[H1]	0.35	
K_{NO_2d}	M-M constant for reduction of NO ₂ ⁻ by denitrifiers	g N m ⁻³	[H8]	3.5	Yoshinari et al. (1977)
K_{NO_2n}	M-M constant for reduction of NO ₂ ⁻ by nitrifiers	g N m ⁻³	[H20]	3.5	
K_{NO_2o}	M-M constant for oxidation of NO ₂ ⁻ by nitrifiers	g N m ⁻³	[H15]	10	
K_{NO_3d}	M-M constant for reduction of NO ₃ ⁻ by denitrifiers	g N m ⁻³	[H7]	3.5	Yoshinari et al. (1977)
K_{N_2Od}	M-M constant for reduction of N ₂ O by denitrifiers	g N m ⁻³	[H9]	0.35	Yoshinari et al. (1977)
K_{O_2h}	M-M constant for reduction of O _{2s} by heterotrophs	g O ₂ m ⁻³	[H4b]	0.32	Griffin (1972)
K_{O_2n}	M-M constant for reduction of O _{2s} by NH ₃ oxidizers	g O ₂ m ⁻³	[H13b]	0.32	Focht and Verstraete (1977)
K_{O_2o}	M-M constant for reduction of O _{2s} by NO ₂ ⁻ oxidizers	g O ₂ m ⁻³	[H17b]	0.32	Focht and Verstraete (1977)

K_{xh}	M-M constant for oxidation of DOC by heterotrophs	g C m^{-3}	[H2]	12	(McGill et al., 1981)
$M_{i,h,a}$	active biomass of heterotrophs	g C m^{-2}	[H2,H7]		
$M_{i,n,a}$	active biomass of NH_3 oxidizers	g C m^{-2}	[H11,H13]		
$M_{i,m,j,C}$	C biomass of microbial population $M_{i,m,j}$	g C m^{-2}	[H1]		
$M_{i,m,j,N}$	N biomass of microbial population $M_{i,m,j}$	g N m^{-2}	[H1]		
$M_{i,o,a}$	active biomass of NO_2^- oxidizers	g C m^{-2}	[H15,H17]		
$[\text{NH}_{3s}]$	concentration of NH_3 in soil solution	g N m^{-3}	[H11]		
$[\text{NH}_4^+]$	concentration of NH_4^+ in soil solution	g N m^{-3}	[H1]		
$[\text{NO}_2^-]$	concentration of NO_2^- in soil solution	g N m^{-3}	[H8,H15,H20]		
$[\text{NO}_3^-]$	concentration of NO_3^- in soil solution	g N m^{-3}	[H7]		
$[\text{N}_2\text{O}]$	concentration of N_2O in soil solution	g N m^{-3}	[H9]		
n	number of microbes	g^{-1}	[H13,H17]		
$[\text{O}_{2mi,h}]$	O_2 concentration at heterotrophic surfaces	$\text{g O}_2 \text{ m}^{-3}$	[H7]		
$[\text{O}_{2mi,n}]$	O_2 concentration at NH_3 oxidizer surfaces	$\text{g O}_2 \text{ m}^{-3}$	[H13]		
$[\text{O}_{2mi,o}]$	O_2 concentration at NO_2^- oxidizer surfaces	$\text{g O}_2 \text{ m}^{-3}$	[H17]		
$[\text{O}_{2s}]$	O_2 concentration in soil solution	$\text{g O}_2 \text{ m}^{-3}$	[H7,H13,H17]		
$R_{\text{NO}_2i,d}$	NO_2^- reduction by denitrifiers	$\text{g N m}^{-2} \text{ h}^{-1}$	[H8,H9,H10]		
$R'_{\text{NO}_2i,n}$	rate of NO_2^- reduction by NH_3 oxidizers under non-limiting $[\text{NO}_2^-]$ and $[\text{CO}_{2s}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H19,H20]		
$R_{\text{NO}_2i,n}$	rate of NO_2^- reduction by NH_3 oxidizers under ambient $[\text{NO}_2^-]$ and $[\text{CO}_{2s}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H20,H21]		
$R'_{\text{NO}_3i,d}$	NO_3^- reduction by denitrifiers under non-limiting $[\text{NO}_3^-]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H6,H7,H8,H9]		
$R_{\text{NO}_3i,d}$	NO_3^- reduction by denitrifiers under ambient $[\text{NO}_3^-]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H7,H8,H9,H10]		
$R_{\text{N}_2\text{O}i,d}$	N_2O reduction by denitrifiers	$\text{g N m}^{-2} \text{ h}^{-1}$	[H9,H10]		
$R'_{\text{O}_2i,d}$	rate of O_{2s} reduction by denitrifiers under non-limiting $[\text{O}_{2s}]$	$\text{g O}_2 \text{ m}^{-2} \text{ h}^{-1}$	[H6]		
$R_{\text{O}_2i,d}$	rate of O_{2s} reduction by denitrifiers under ambient $[\text{O}_{2s}]$	$\text{g O}_2 \text{ m}^{-2} \text{ h}^{-1}$	[H6]		

$R'_{O_2i,h}$	rate of O_{2S} reduction by heterotrophs under non-limiting [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H3,H4,H5]		
$R_{O_2i,h}$	rate of O_{2S} reduction by heterotrophs under ambient [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H4,H5]		
$R'_{O_2i,n}$	rate of O_{2S} reduction by NH_3 oxidizers under non-limiting [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H12,H13,H14,H19]		
$R_{O_2i,n}$	rate of O_{2S} reduction by NH_3 oxidizers under ambient [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H13,H14,H19]		
$R'_{O_2i,o}$	rate of O_{2S} reduction by NO_2^- oxidizers under non-limiting [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H16,H17,H18]		
$R_{O_2i,o}$	rate of O_{2S} reduction by NO_2^- oxidizers under ambient [O_{2S}]	$g\ O_2\ m^{-2}\ h^{-1}$	[H17,H18]		
RQ_C	respiratory quotient for reduction of O_2 coupled to oxidation of C	$g\ O_2\ g\ C^{-1}$	[H3,H12,H16]	2.67	Brock and Madigan (1991)
RQ_{NH₃}	respiratory quotient for reduction of O_2 coupled to oxidation of NH_3	$g\ O_2\ g\ N^{-1}$	[H12]	3.43	Brock and Madigan (1991)
RQ_{NO₂}	respiratory quotient for reduction of O_2 coupled to oxidation of NO_2^-	$g\ O_2\ g\ N^{-1}$	[H16]	1.14	Brock and Madigan (1991)
r_m	radius of microbial sphere	m	[H4,H13,H17]		
r_w	radius of r_m + water film at current soil water potential	m	[H4,H13,H17]		from ψ_s according to Kemper (1966)
$X'_{Ci,n}$	rate of C oxidation by NH_3 oxidizers under non-limiting [O_{2S}]	$g\ C\ m^{-2}\ h^{-1}$	[H12]		
$X'_{Ci,o}$	rate of C oxidation by NO_2^- oxidizers under non-limiting [O_{2S}]	$g\ C\ m^{-2}\ h^{-1}$	[H16]		
X'_{DOC}	specific rate of DOC oxidation by heterotrophs at 25 °C under non-limiting [DOC] and [O_{2S}]	$g\ C\ g\ C^{-1}\ h^{-1}$	[H2]	0.125	Shields et al. (1973)
$X'_{DOCi,h}$	rate of DOC oxidation by heterotrophs under non-limiting [O_{2S}]	$g\ N\ m^{-2}\ h^{-1}$	[H2,H3,H5]		
$X_{DOCi,h}$	rate of DOC oxidation by heterotrophs under ambient [O_{2S}]	$g\ N\ m^{-2}\ h^{-1}$	[H5]		

$X_{\text{DOC},i,d}$	rate of DOC oxidation by heterotrophs under ambient $[\text{O}_{2\text{S}}]$ and $[\text{NO}_x]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H10]		
X'_{NH_3}	specific rate of NH_3 oxidation by NH_3 oxidizers at 25 °C under non-limiting $[\text{O}_{2\text{S}}]$	$\text{g N g C}^{-1} \text{ h}^{-1}$	[H11]]	0.625	Belser and Schmidt (1980)
$X_{\text{NH}_3,i,n}$	rate of NH_3 oxidation by NH_3 oxidizers coupled with reduction of $\text{O}_2 + \text{NO}_2^-$ under ambient $[\text{O}_{2\text{S}}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H14,H21]		
$X'_{\text{NH}_3,i,n}$	rate of NH_3 oxidation by NH_3 oxidizers under non-limiting $[\text{O}_{2\text{S}}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H11,H12,H14]		
$X'_{\text{NO}_2,i,o}$	rate of NO_2^- oxidation by NO_2^- oxidizers under non-limiting $[\text{O}_{2\text{S}}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H15,H16,H18]		
$X_{\text{NO}_2,i,o}$	rate of NO_2^- oxidation by NO_2^- oxidizers coupled with reduction of O_2 under ambient $[\text{O}_{2\text{S}}]$	$\text{g N m}^{-2} \text{ h}^{-1}$	[H18]		
X'_{NO_2}	specific rate of NO_2^- oxidation by NO_2^- oxidizers at 25 °C under non-limiting $[\text{O}_{2\text{S}}]$	$\text{g N g C}^{-1} \text{ h}^{-1}$	[H15]	2.5	Belser (1977)

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