SUPPLEMENTARY MATERIAL

Model development

General

Ecosys is an hourly time-step model with multiple canopy and soil layers that provide a framework for different plant and microbial populations to acquire, transform and exchange resources (energy, water, C, N and P). The model is constructed from algorithms representing basic physical, chemical and biological processes that determine process rates in plant and microbial populations interacting within complex biomes. These algorithms interact to simulate complex ecosystem behaviour across a wide range of spatial and biological scales. The model is designed to represent terrestrial ecosystems under range of natural and anthropogenic disturbances and environmental changes at patch (spatially homogenous one-dimensional) and landscape (spatially variable two- or three-dimensional) scales. A comprehensive description of *ecosys* with a detailed listing of inputs, outputs, governing equations, parameters, results and references can be found in Grant (2001). A more detailed description of model algorithms and parameters most relevant to simulating temperature, water and nutrient effects on net ecosystem productivity (NEP) is given below, with reference to equations and variable definitions in appendices A-H 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 soil temperature (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. 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 and senescence* below. 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 and senescence* below. 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 ($\boldsymbol{R_m}$) [A18, A19], depending on microbial N and T_s as described earlier for plants. R_h in excess of $\boldsymbol{R_m}$ 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 $\boldsymbol{R_h}$ causes microbial dieback. M also undergoes first-order decomposition ($\boldsymbol{D_m}$) [A23]. Internal retention and recycling of microbial N and P during decomposition [A24] is modelled whenever these nutrients constrain R_h [A12]. Changes in *M* arise from differences between gains from DOC uptake and losses from $R_m + R_g + D_m$ [A25].

Microbial nutrient exchange

During these changes, all microbial populations seek to maintain set minimum ratios of C:N or C:P in *M* by mineralizing or immobilizing NH_4^+, NO_3^- and $H_2PO_4^-$ [A26], thereby controlling solution $[NH_4^+]$, $[NO_3^-]$ and $[H_2PO_4^-]$ that determine root and mycorrhizal uptake. 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 *C_3 gross primary productivity* when ψ_c is solved in the second stage of the convergence solution. 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 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, 1998a).

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 in *Canopy transpiration* is recalculated for each adjusted value of ψ_c during convergence.

Appendix C: Gross primary productivity and autotrophic respiration

C_3 gross primary productivity

After successful convergence for T_c and ψ_c as described in *Canopy transpiration*, 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_lmin at zero ψ_c [C5] to r_c at ambient ψ_c [C4], and by non-stomatal effects(f_ψ) [C9] on CO_2- and light-limited carboxylation (V_b) [C6] and V_j [C7] (Grant and Flanagan, 2007). The recalculation of V_c is accomplished through a convergence solution for C_i and its aqueous counterpart C_c at which V_g [C2] equals V_c [C3] (Grant and Flanagan, 2007). The CO_2 fixation rate of each leaf surface at convergence is added to arrive at a value for gross primary productivity (GPP) by each plant population in the model [C1]. The CO_2 fixation product is stored in nonstructural C pools (σ_C) in each branch.

GPP is strongly controlled by nutrient uptake (U_{NH_4}, U_{NO_3} and U_{PO_4} [C23]), products of which are added to nonstructural N (σ_N) and P (σ_P) in root and mycorrhizal layers where they are coupled with σ_C to drive growth of branches, roots and mycorrhizae as described in *Growth and senescence*. Low σ_N:σ_C or σ_P:σ_C in branches indicate excess CO_2 fixation with respect to N or P uptake for phytomass growth. Such ratios in the model have two effects on GPP:

(1) They reduce activities of rubisco [C6a] and chlorophyll [C7a] through product inhibition [C11], thereby simulating the suppression of CO_2 fixation by leaf σ_C accumulation widely reported in the literature.

(2) They reduce the structural N:C and P:C ratios at which leaves are formed because σ_C, σ_N and σ_P are the substrates for leaf growth. Lower structural ratios cause a proportional reduction in areal concentrations of rubisco [C6b] and chlorophyll [C7b], reducing leaf CO_2 fixation.

Autotrophic respiration

The temperature dependent oxidation of these nonstructural pools (R_c) [C14], plus the energy costs of nutrient uptake [C23], drive autotrophic respiration (R_a) [C13] by all branches, roots and mycorrhizae. R_c by roots and mycorrhizae is constrained by O_2 uptake (U_{O2}) [C14b] calculated by solving for aqueous O_2 concentrations at root and mycorrhizal surfaces ([O_{2r}]) at which convection + radial diffusion through the soil aqueous phase plus radial diffusion through the root aqueous phase [C14d] equals active uptake driven by O_2 demand from R_c [C14c] (Grant, 2004). These diffusive fluxes are in turn coupled to volatilization -dissolution between aqueous and gaseous phases in soil and root [D14]. The diffusion processes are driven by aqueous O_2 concentrations sustained by transport and dissolution of gaseous O_2 through soil and roots (Grant, 2004), and are governed by lengths and surface areas of roots and mycorrhizae (Grant, 1998a). Thus R_c is coupled to O_2 reduction by all root and mycorrhizal populations according to O_2 availability. R_c is first used to meet maintenance respiration requirements (R_m), calculated independently of R_c from the N content in each organ, and a function of T_c or T_s [C16]. Any excess of R_c over R_m is expended as growth respiration (R_g), constrained by branch, root or mycorrhizal ψ_t [C17]. When R_m exceeds R_c, the shortfall is met by the respiration of remobilizable C (R_s) in leaves and twigs or roots and mycorrhizae [C15].

Growth and senescence

R_g drives the conversion of branch σ_C into foliage, twigs, branches, boles and reproductive material according to organ growth yields (Y_g) and phenology-dependent partitioning coefficients [C20], and the conversion of root and mycorrhizal σ_C into primary and secondary axes according to root and mycorrhizal growth yields. Growth also requires organ-specific ratios of nonstructural N (σ_N) and P (σ_P) from U_{NH4}, U_{NO3} and U_{PO4} [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, 1998a). Low σ_{N}:σ_{C} or σ_{P}:σ_{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 σ_{N}:σ_{C} or σ_{P}:σ_{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]. Provision is also made to withdraw remobilizable N or P from leaves and twigs or roots and mycorrhizae when ratios of σ_N:σ_C or σ_P:σ_C become smaller than those required for growth of new phytomass. This withdrawal drives the withdrawal of associated remobilizable C, and the loss of associated non-remobilizable C, N and P as litterfall. Environmental constraints such as water, heat, nutrient or O_2 stress that reduce σ_C and hence R_c with respect to R_m therefore hasten litterfall.

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

Root and mycorrhizal nutrient uptake

Root and mycorrhizal uptake of N and P ($U_{\mathrm{NH_4}}$, $U_{\mathrm{NO_3}}$ and $U_{\mathrm{PO_4}}$) 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 $U_{\mathrm{NH_4}}$, $U_{\mathrm{NO_3}}$ and $U_{\mathrm{PO_4}}$ 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, 1998a). A product inhibition function is included to avoid uptake in excess of nutrient requirements [C23g].

C_4 gross primary productivity

C_4 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 C_4 product inhibition (Jiao and Chollet, 1988; Lawlor, 1993) [C34], ψ_c ([C35] as described in Grant and Flanagan (2007)) and T_c [C36]. Leaf surface N density is controlled by leaf structural N:C and P:C ratios calculated during leaf growth from leaf non-structural N:C and P:C ratios arising from root N and P uptake (Grant, 1998a) vs. CO_2 fixation.

C_4 mesophyll-bundle sheath exchange

Differences in the mesophyll and bundle sheath concentrations of the C_4 carboxylation product drive mesophyll-bundle sheath transfer (Leegood, 2000) [C37]. The bundle sheath concentration of the C_4 product drives a product-inhibited decarboxylation reaction (Laisk and Edwards, 2000) [C38], the CO_2 product of which generates a concentration gradient that drives leakage of CO_2 from the bundle sheath to the mesophyll [C39]. CO_2 in the bundle sheath is maintained in 1:50 equilibrium with HCO_3^- (Laisk and Edwards, 2000). At this stage of model development, the return of a C_3 decarboxylation product from the bundle sheath to the mesophyll is not simulated. Parameters used in Eqs. [C37-C39] allowed mesophyll and bundle sheath concentrations of C_4 carboxylation products from [C40-C41] to be maintained at values consistent with those in Leegood (2000), bundle sheath concentrations of CO_2 (from [C42]) to be maintained at values similar to those reported by Furbank and Hatch (1987), and bundle sheath CO_2 leakiness [C39]), expressed as a fraction of PEP carboxylation, to be maintained at values similar to those in Williams et al. (2001), in sorghum as described in Grant et al. (2004).

C_4 bundle sheath

A C_3 model in which carboxylation is the lesser of CO_2- and light-limited reaction rates (Farquhar et al., 1980) has been parameterized for the bundle sheath of C_4 plants [C43] from Seeman et al. (1984). The CO_2-limited rate [C44] is a Michaelis-Menten function of RuBP carboxylase (RuBPc) activity and bundle sheath CO_2 concentration

[C42]. The light-limited rate [C45] is a hyperbolic function of absorbed irradiance and activity of chlorophyll associated with the bundle sheath with a quantum yield based on 3 ATP [C46]. The provision of reductant from the mesophyll to the bundle sheath in NADP-ME species is not explicitly simulated. RuBPc [C47] and chlorophyll [C48] activities are the products of specific activities and concentrations multiplied by set fractions of leaf surface N density, and from functions of C_3 product inhibition (Bowes, 1991; Stitt, 1991] [C49], ψ_c ([A12] from Grant and Flanagan (2007)) and T_c [C36].

Rates of C_3 product removal are controlled by phytomass biosynthesis rates driven by concentrations of nonstructural products from leaf CO_2 fixation and from root N and P uptake. If biosynthesis rates are limited by nutrient uptake, consequent depletion of nonstructural N or P and accumulation of nonstructural C will constrain specific activities of RuBP and chlorophyll [C47-C49], and thereby slow C_3 carboxylation [C43], raise bundle sheath CO_2 concentration [C42], accelerate CO_2 leakage [C39], slow C_4 decarboxylation [C38], raise C_4 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.

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

Exchange with water table

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

Surface heat flux

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

Gas flux

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

Solute flux

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

Appendix E: Solute transformations

Precipitation-dissolution equilibria

Solution [NH_4^+], [NO_3^-] and [$H_2PO_4^-$] that drive U_{NH4}, U_{NO3} and U_{PO4} [C23] are controlled by precipitation, adsorption and ion pairing reactions (Grant and Heaney, 1997; Grant et al., 2004), including precipitation-dissolution of $Al(OH)_3$, $Fe(OH)_3$, $CaCO_3$, $CaSO_4$, $AlPO_4$, $FePO_4$, $Ca(H_2PO_4)_2$, $CaHPO_4$, and $Ca_5(PO_4)_3OH$ [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: N_2 fixation

Rhizobial growth

Modelling the activity of symbiotic N_2 fixing bacteria in roots follows a protocol similar to that of non-symbiotic N_2 fixing bacteria in soil. Respiration demand is driven by specific activity, microbial biomass (M_n), and nonstructural C concentration ($[\chi_n]$) in root nodules [F1], and is constrained by temperature [F2] and microbial N or P status [F3]. Nodule respiration (R) is constrained by the extent to which O_2 uptake meets O_2 demand [F4] imposed by respiration demand [F5]. O_2 uptake is in turn constrained by rhizosphere $[O_{2r}]$ [F6a] which is controlled by radial diffusion of O_2 through soil water to roots and nodules [F6b]. Soil water $[O_2]$ is maintained by dissolution of O_2 from soil air which is in turn maintained by soil-atmosphere gas exchange and vertical diffusion (Grant, 2004). R_h is first allocated to maintenance respiration R_m [F7-F8] and the remainder if any is allocated to growth respiration R_g [F9]. If R_m exceeds R_h, the shortfall is made up from respiration of microbial protein C, forcing senescence and litterfall of associated non-protein C [F10-F11].

N_2 fixation

N_2 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 nodule [F13]. ν_n is the product of $V_{\mathrm{N_2}}$, so that [F12] simulates the inhibition of N_2 fixation by its product (Postgate, 1998). The value of $V_{\mathrm{N_2}}$ is also limited by the additional N needed to maintain bacterial N content [N_n'] of M_n [F12], so that N_2 fixation is constrained by the need of nodule bacteria for N not met from other sources (Postgate, 1998). Respiration required for N_2 fixation $R_{\mathrm{N_2}}$ [F14] is subtracted from R_g [F15] when calculating microbial growth [F16-F18]. Microbial senescence drives N and P litterfall [F19-F20].

Nodule-root exchange

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

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

Appendix G: CH_4 production and consumption

Anaerobic fermenters and H_2 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 ($M_{i,n,a}$) [G1-G7] (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 [G11] (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 [G1]. Respiration products are partitioned among $A_{i,c}$, CO_2 and H_2 according to Brock and Madigan (1991) [G2]. $R_{i,f}$ beyond that used for maintenance respiration drives the uptake of additional $DOC_{i,c}$[G3] for microbial growth according to the growth yield (Y_f) from fermentation [G4]. The growth yield from fermentation is calculated by dividing the free energy change of fermentation, adjusted for H_2 product concentration [G5], by the energy required to transform soluble organic C into microbial C [G4]. Change in $M_{i,f,j}$ is thus the difference between uptake and respiration of $DOC_{i,c}$, less decomposition [G6]. This change determines $M_{i,f,a}$ used in the following calculation of $R_{i,f}$ [G1]. Ratios of $M_{i,f,j,c}$ to $M_{i,f,j,n}$ determine mineralization-immobilization of N [G23] (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) [G26-G28] (Grant et al., 1993a) which undergo further hydrolysis.

Acetotrophic methanogens

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

Hydrogenotrophic methanogens

The fermenter products CO_2 and H_2 [G2] are the substrates for CO_2 reduction by hydrogenotrophic methanogens ($n = h$) which are assumed to be autotrophic [G12]. Respiration products are partitioned between CH_4 and H_2O according to Brock and Madigan (1991) [G13]. R_h beyond that used for maintenance respiration drives the uptake of additional CO_2 [G14] for microbial growth according to the growth yield (Y_h) of hydrogenotrophic methanogenesis (Brock and Madigan, 1991) [G15]. This growth yield is calculated by dividing the free energy change of hydrogenotrophic methanogenesis, adjusted for H_2 substrate concentration [G16], by the energy required to transform CO_2 into microbial C. Change in $M_{h,j}$ is thus the difference between uptake and respiration of CO_2, less decomposition [G17]. This change determines $M_{h,a}$ used in the following calculation of R_h [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 ($n = t$) [G18]. The stoichiometry and energetics of the methanotrophic reactions [G22-G24] are based on those of CH_4 to CO_2 in Brock and Madigan (1991). The oxidation of CH_4 to CO_2 is coupled through an energy yield with the oxidation of CH_4 to organic C used in microbial respiration [G19]. The energy yield from CH_4 oxidation is calculated by dividing the free energy change of CH_4 oxidation by the energy required to transform CH_4 into organic C [G20]. Oxygen requirements to sustain CH_4 oxidation rates are then calculated from the stoichiometries of CH_4 oxidation [G22-G23] and aerobic microbial respiration [G24]. The O_2 concentrations at methanotrophic microsites are then found at which active O_2 uptake driven by requirements for CH_4 oxidation equals spherical O_2 diffusion to the microsites from the soil solution. 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 and Rochette, 1994; Grant, 1995], 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_{O_2t}) is then used to constrain

CH_4 oxidation rates [G21] so that CH_4 oxidation is stoichiometrically coupled to O_2 uptake. Growth respiration by methanotrophs is calculated as the difference between total respiration (R_t) from eq. [G21b] and maintenance respiration (R_{mt}) from eqs. [G18-G19] (Grant et al., 1993a). Growth respiration drives the uptake and transformation of additional CH_4 into microbial biomass ($M_{t,c}$) [G25]) according to the growth yield. This yield is calculated by dividing the free energy change of CH_4 oxidation (Brock and Madigan, 1991) [G18] by the energy required to construct new microbial biomass from CH_4 [G26]. Net growth of the methanotrophic population $M_{t,j,c}$ is calculated as the uptake of CH_4-C minus respiration and decomposition of assimilated C [G27]. This change determines $M_{t,a}$ used in the following calculation of X'_t [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-G27] 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 NH_4^+ 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 O_2 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 [H7-H13] 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 NO_3^-, NO_2^- and N_2O 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 NH_3 and reduction of O_2 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 $M_{i,n}$ according to construction energy costs of each nitrifier population [H32-H34] in Grant and Pattey (2003).

Oxidation of NO_2^- and reduction of O_2 by nitrifiers

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

Oxidation of NH_3 and reduction of NO_2^- 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 $M_{i,n}$.

Equations and definitions of variables

Appendix A: Soil C, N and P transformations

Decomposition

$D_{Si,j,l,\mathrm{C}} = D'_{Si,j,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\ \ f_{\mathrm{tg}l}\,(S_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of litter, POC, humus	[A1a]
$D_{Zi,j,l,\mathrm{C}} = D'_{Zi,j,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\ f_{\mathrm{tg}l}\,(Z_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of microbial residues	[A1b]
$D_{Ai,l,\mathrm{C}} = D'_{Ai,l,\mathrm{C}}\, M_{i,d,l,\mathrm{C}}\ f_{\mathrm{tg}l}\,(A_{i,l,\mathrm{C}} / G_{i,l,\mathrm{C}})$	decomposition of adsorbed SOC	[A1c]
$S_{i,l,\mathrm{C}} = \Sigma_j\, S_{i,j,l,\mathrm{C}}$	total C in all kinetic components of litter, POC, humus	[A2a]
$Z_{i,l,\mathrm{C}} = \Sigma_j\, Z_{i,j,l,\mathrm{C}}$	total C in all kinetic components of microbial residues	[A2b]
$G_{i,l,\mathrm{C}} = S_{i,l,\mathrm{C}} + Z_{i,l,\mathrm{C}} + A_{i,l,\mathrm{C}}$	total C in substrate-microbe complexes	[A2c]

$$M_{i,d,l,\mathrm{C}} = M_{i,a,l,\mathrm{C}} + \boldsymbol{q_m}\,(M_{i,a,l,\mathrm{C}}\,G_{ix,l,\mathrm{C}} - M_{ix,a,l,\mathrm{C}}\,G_{i,l,\mathrm{C}})/(G_{ix,l,\mathrm{C}} + G_{i,l,\mathrm{C}}) \tag{A3a}$$

$$M_{i,a,l,\mathrm{C}} = \Sigma_n\,M_{i,n,a,l,\mathrm{C}} \tag{A3b}$$

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

$$D'_{Si,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Sj,\mathrm{C}}[S_{i,j,l,\mathrm{C}}]\}/\{[S_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [\Sigma M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\} \tag{A4a}$$

$$D'_{Zi,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Zj,\mathrm{C}}[Z_{i,j,l,\mathrm{C}}]\}/\{[Z_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\} \tag{A4b}$$

$$D'_{Ai,l,\mathrm{C}} = \{\boldsymbol{D}_{A,\mathrm{C}}[A_{i,l,\mathrm{C}}]\}/\{[A_{i,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}(1.0 + [M_{i,d,l,\mathrm{C}}]/\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\} \tag{A4c}$$

substrate and water constraint on *D* from colonized litter, POC and humus, microbial residues and adsorbed SOC

$$\delta S_{i,j,k,l,\mathrm{C}}/\delta t = \boldsymbol{\beta}\,\Sigma_n\,(U_{i,n,l\mathrm{C}} - R_{\mathrm{h}i,n,l})\,(S'_{i,j,k,l,\mathrm{C}}/\,S'_{i,j,l,\mathrm{C}})\,\{(S'_{i,j,l,\mathrm{C}}/S_{i,j,l,\mathrm{C}})/(\,S'_{i,j,l,\mathrm{C}}/S_{i,j,l\,,\mathrm{C}} + \boldsymbol{K}_{\mathbf{i}\boldsymbol{S}})\} \tag{A5}$$

colonized litter determined by microbial growth into uncolonized litter

$$f_{\mathrm{tg}l} = T_{\mathrm{s}l}\{e^{[B - \boldsymbol{H}_{\mathbf{a}}/(\boldsymbol{R}T_{\mathrm{s}l})]}\}/\{1 + e^{[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{s}l})/(\,\boldsymbol{R}T_{\mathrm{s}l})]} + e^{[(\boldsymbol{S}T_{\mathrm{s}l} - \boldsymbol{H}_{\mathbf{dh}})/(\,\boldsymbol{R}T_{\mathrm{s}l})]}\} \tag{A6}$$

Arrhenius function for *D* and R_h

$D_{Si,j,l,\mathrm{N,P}} = D_{Si,j,l,\mathrm{C}}(S_{i,j,l,\mathrm{N,P}}/S_{i,j,l,\mathrm{C}})$	N and P coupled with C during D	[A7a]
$D_{Zi,j,l,\mathrm{N,P}} = D_{Zi,j,l,\mathrm{C}}(Z_{i,j,l,\mathrm{N,P}}/Z_{i,j,l,\mathrm{C}})$		[A7b]
$D_{Ai,l,\mathrm{N,P}} = D_{Ai,l,\mathrm{C}}(A_{i,l,\mathrm{N,P}}/A_{i,l,\mathrm{C}})$		[A7c]
$Y_{i,l,\mathrm{C}} = \boldsymbol{k}_{\mathbf{ts}}(G_{i,l,C}\, F_{\mathrm{s}}[Q_{i,l,\mathrm{C}}]^{\boldsymbol{b}} - X_{i,l,\mathrm{C}})$	Freundlich sorption of DOC	[A8]
$Y_{i,l,\mathrm{N,P}} = Y_{i,l,\mathrm{C}}(Q_{i,l,\mathrm{N,P}}/Q_{i,l,\mathrm{C}})$	$(Y_{i,l,\mathrm{C}} > 0)$ adsorption of DON, DOP	[A9]
$Y_{i,l,\mathrm{N,P}} = Y_{i,l,\mathrm{C}}(X_{i,l,\mathrm{N,P}}/X_{i,l,\mathrm{C}})$	$(Y_{i,l,\mathrm{C}} < 0)$ desorption of DON, DOP	[A10]

Microbial growth

$R_{\mathrm{h}} = \Sigma_i \Sigma_n \Sigma_l R_{\mathrm{h}i,n,l}$		[A11]
$\boldsymbol{R}_{\mathrm{h}i,n,l} = \boldsymbol{R'}_{\mathrm{h}n} \min\{C_{\mathrm{N}i,n,l,a}/\boldsymbol{C}_{\mathbf{N}j}, C_{\mathrm{P}i,n,l,a}/\boldsymbol{C}_{\mathbf{P}j}\}$	R_{h} constrained by microbial N, P	[A12]
$R_{\mathrm{h}}'{}_{i,n,l} = M_{i,n,a,l,\mathrm{C}}\, \{\boldsymbol{R}_{\mathrm{h}i,n,l}\, [Q_{i,l,\mathrm{C}}]\}/\{(\boldsymbol{K}_{\mathbf{m}\boldsymbol{Q}\mathbf{C}} + [Q_{i,l,\mathrm{C}}])\} f_{\mathrm{tg}l}\, f_{\psi\mathrm{g}l}$	R_{h} constrained by substrate DOC	[A13]
$R_{\mathrm{h}i,n,l} = R_{\mathrm{h}}'{}_{i,n,l}\, (U_{\mathrm{O2}i,n,l}/U'_{\mathrm{O2}i,n,l})$	R_{h} constrained by O_2	[A14]
$f_{\psi\mathrm{g}l} = 1.0 - 6.67(1.0 - e^{(M\psi_{\mathrm{s}}/(\boldsymbol{R}T_{\mathrm{s}l})})$	ψ_{s} constraints on microbial growth	[A15]

$U'_{\mathrm{O2}i,n,l} = 2.67R_{\mathrm{h}}'_{i,n,l}$	O_2 demand driven by potential R_{h}	[A16]
$U_{\mathrm{O2}i,n,l} = U'_{\mathrm{O2}i,n,l}[\mathrm{O}_{2\mathrm{m}i,n,l}]/([\mathrm{O}_{2\mathrm{m}i,n,l}] + \boldsymbol{K}_{\mathbf{O_2}})$	active uptake coupled with radial diffusion of O_2	[A17a]
$= 4\pi n\, M_{i,n,a,l,\mathrm{C}}\, D_{\mathrm{sO2}l}[\boldsymbol{r}_{\mathbf{m}} r_{\mathrm{w}l}/(r_{\mathrm{w}l} - \boldsymbol{r}_{\mathbf{m}})]([\mathrm{O}_{2\mathrm{s}l}] - [\mathrm{O}_{2\mathrm{m}i,n,l}]$		[A17b]
$R_{\mathrm{m}i,n,j,l} = \boldsymbol{R}_{\mathrm{m}} M_{i,n,j,l,\mathrm{N}}\, f_{\mathrm{tm}l}$		[A18]
$f_{\mathrm{tm}l} = e^{[\boldsymbol{y}(T_{\mathrm{s}l} - 298.16)]}$		[A19]
$R_{\mathrm{g}i,n,l} = R_{\mathrm{h}i,n,l} - \Sigma_j R_{\mathrm{m}i,n,j,l}$		[A20]
$U_{i,n,l\mathrm{C}} = \min(R_{\mathrm{h}i,n,l}, \Sigma_j R_{\mathrm{m}i,n,j,l}) + R_{\mathrm{g}i,n,l}(1 + \boldsymbol{\Delta G}/\boldsymbol{E}_{\mathbf{m}})$	DOC uptake driven by R_{g}	[A21]
$U_{i,n,l\mathrm{N,P}} = U_{i,n,l}Q_{i,l,\mathrm{N,P}}/Q_{i,l,\mathrm{C}}$	DON,DOP uptake driven by $U_{i,n,l\mathrm{C}}$	[A22]
$D_{Mi,n,j,l,\mathrm{C}} = \boldsymbol{D}_{Mi,j} M_{i,n,j,\mathrm{C}}\, f_{\mathrm{tg}}$	first-order decay of microbial C,	[A23]
$D_{Mi,n,j,\mathrm{N,P}} = \boldsymbol{D}_{Mi,j} M_{i,n,j,l,\mathrm{N,P}}\, f_{\mathrm{tg}l}\, f_{\mathrm{d}i,n,l\mathrm{N,P}}$	partial release of microbial N, P	[A24]
$\delta M_{i,n,j,l,\mathrm{C}}/\delta t = F_j U_{i,n,l\mathrm{C}} - F_j R_{\mathrm{h}i,n,l} - D_{Mi,n,j,l,\mathrm{C}}$	$[R_{\mathrm{h}i,n,l} > R_{\mathrm{m}i,n,j,l}]$ growth	[A25a]
$\delta M_{i,n,j,l,\mathrm{C}}/\delta t = F_j U_{i,n,l\mathrm{C}} - R_{\mathrm{m}i,n,j,l} - D_{Mi,n,j,l,\mathrm{C}}$	$[R_{\mathrm{h}i,n,l} < R_{\mathrm{m}i,n,j,l}]$ senescence	[A25b]

Microbial nutrient exchange

$U_{\mathrm{NH4}i,n,j,l} = (M_{i,n,j,l,C}\,\boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - M_{i,n,j,l,N})$	$U_{\mathrm{NH}_4} < 0$	mineralization	[A26a]
$U_{\mathrm{NH}_4 i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - M_{i,n,j,l,N}),$ $\boldsymbol{U'}_{\mathbf{NH_4}}\, a_{i,n,j,l}\ ([\mathrm{NH}_4{}^{+}{}_{i,n,j,l}]-[\mathbf{NH_4{}^{+}{}_{mn}}])/([\mathrm{NH}_4{}^{+}{}_{i,n,j,l}]-[\mathbf{NH_4{}^{+}{}_{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\}$	$U_{\mathrm{NH}_4} > 0$	immobilization	[A26b]
$U_{\mathrm{NO}_3 i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - (M_{i,n,j,l,N} + U_{\mathrm{NH}_4 i,n,j,l}))\ ,$ $\boldsymbol{U'}_{\mathbf{NO_3}}\, a_{i,n,j,l}\ ([\mathrm{NO}_3{}^{-}{}_{i,n,j,l}]-[\mathbf{NO_3{}^{-}{}_{mn}}])/([\mathrm{NO}_3{}^{-}{}_{i,n,j,l}]-[\mathbf{NO_3{}^{-}{}_{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\}$	$U_{\mathrm{NO}_3} > 0$	immobilization	[A26c]
$U_{\mathrm{PO4}i,n,j,l} = (M_{i,n,j,l,C}\,\boldsymbol{C}_{\mathbf{P}\boldsymbol{j}} - M_{i,n,j,l,P})$	$U_{\mathrm{PO}_4} < 0$	mineralization	[A26d]
$U_{\mathrm{PO4}i,n,j,l} = \min\{(M_{i,n,j,l,C}\,\boldsymbol{C}_{\mathbf{P}\boldsymbol{j}} - M_{i,n,j,l,P}),$ $\boldsymbol{U'}_{\mathbf{PO_4}}\, A_{i,n,j,l}\ \mathbf{(}[\mathrm{H_2PO_4}{}^{-}{}_{i,n,j,l}]\mathbf{-[H_2PO_4{}^{-}{}_{mn}])/(}[\mathrm{H_2PO_4}{}^{-}{}_{i,n,j,l}]\mathbf{-[\ H_2PO_4{}^{-}{}_{mn}] +} \boldsymbol{K}_{\mathbf{PO_4}}\mathbf{)\}}$	$U_{\mathrm{PO}_4} > 0$	immobilization	[A26e]
$\Phi_{i,n=f,j,l} = max\{0,\ M_{i,n=f,j,l,\mathrm{C}}\boldsymbol{C}_{\mathbf{N}j} - M_{i,n=f,j,l,\mathrm{N}} - max\{0,\ U_{i,n=f,j,l,\mathrm{N}}\}\}$	N_2 fixation driven by N deficit of diazotrophic population		[A27]
$R_{\Phi i,n=f,j,l} = \boldsymbol{E}_{\boldsymbol{\Phi}}\,\Phi_{i,n=f,j,l}$			[A28]

$\delta M_{i,n,j,l,\mathrm{N}}/\delta t = F_j U_{i,n,l,\mathrm{N}} + U_{\mathrm{NH}_{4}i,n,j,l} + U_{\mathrm{NO}_{3}i,n,j,l} + \Phi_{i,n=f,j,l} - D_{Mi,n,j,l,\mathrm{N}}$ growth *vs*. losses of microbial N, P [A29a]

$\delta M_{i,n,j,l,\mathrm{P}}/\delta t = F_j U_{i,n,l,\mathrm{P}} + U_{\mathrm{PO}_{4}i,n,j,l} - D_{Mi,n,j,l,\mathrm{p}}$ [A29b]

$M_{i,n,a,l,\mathrm{C}} = M_{i,n,j=labile,l,\mathrm{C}} + M_{i,n,j=resistant,l,\mathrm{C}} F_{\mathrm{r}}/F_{\mathrm{l}}$ [A30a]

Humification

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

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

$H_{Si,j\neq\mathrm{lignin},l,\mathrm{C}} = H_{Si,j=\mathrm{lignin},l,\mathrm{C}}\, \boldsymbol{L}_{\mathbf{h}j}$ [A33]

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

$H_{Mi,n,j,l,\mathrm{C}} = D_{Mi,n,j,l,\mathrm{C}}\, \boldsymbol{F}_{\mathbf{h}}$ decomposition products of [A35]

$H_{Mi,n,j,l,\mathrm{N,P}} = H_{Mi,n,j,l,\mathrm{C}} M_{i,n,j,l,\mathrm{N,P}}/M_{i,n,j,l,\mathrm{C}}$ microbes added to humus [A36]

depending on clay

Definition of variables in appendix A

Variable	Definition	Unit	Equation	Value	Reference
Subscripts					

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)

Variables

$A_{i,l,\mathrm{C}}$	mass of adsorbed SOC	g C m^{-2}	[A1c,A2c]		
$[A_{i,l,\mathrm{C}}]$	concentration of adsorbed SOC in soil	g C Mg^{-1}	[A4c]		
a	microbial surface area	m^{2} m^{-2}	[A26]		
$\boldsymbol{B}$	parameter such that $f_{\mathrm{tg}} = 1.0$ at $T_l = 298.15$ K		[A6]	26.230	
$\boldsymbol{b}$	Freundlich exponent for sorption isotherm		[A8]	0.85	Grant et al. (1993a, b)
$\boldsymbol{\beta}$	specific colonization rate of uncolonized substrate	-	[A5]	2.5	*Grant et al.* [2010]
$C_{\mathrm{N,P}i,n,a,l}$	ratio of $M_{i,n,a,\mathrm{N,P}}$ to $M_{i,n,a,\mathrm{C}}$	g N or P g C^{-1}	[A12]		

$\boldsymbol{C}_{\mathbf{N,P}j}$	maximum ratio of $M_{i,n,j,\mathrm{N,P}}$ to $M_{i,n,j,\mathrm{C}}$ maintained by $M_{i,n,j,\mathrm{C}}$	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)
$\boldsymbol{D}_{Mi,j}$	specific decomposition rate of $M_{i,n,j}$ at 30°C	g C g C^{-1} h^{-1}	[A23,A24]	0.0125 and 0.00035 for j = labile and resistant, respectively	Grant et al. (1993a, b)
$D_{Mi,n,j,l,\mathrm{C}}$	decomposition rate of $M_{i,n,j,l,\mathrm{C}}$	g C m^{-2} h^{-1}	[A23,A25,A35]		
$D_{Mi,n,j,l,\mathrm{N,P}}$	decomposition rate of $M_{i,n,j,l,\mathrm{N,P}}$	g N or P m^{-2} h^{-1}	[A24,A29]		
$D_{\mathrm{sO2}l}$	aqueous dispersivity–diffusivity of O_2 during microbial uptake in soil	m^{2} h^{-1}	[A17]		
$D_{Ai,l,\mathrm{C}}$	decomposition rate of $A_{i,l,\mathrm{C}}$ by $\boldsymbol{M}_{\boldsymbol{i,d,l},\mathrm{C}}$ producing Q in [A13]	g C m^{-2} h^{-1}	[A1c,A7c,A31c]		
$\boldsymbol{D}_{Aj,\mathrm{C}}$	specific decomposition rate of $A_{i,l,\mathrm{C}}$ by $\boldsymbol{M}_{\boldsymbol{i,d,l},\mathrm{C}}$ at 25°C and saturating[$A_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	[A4c]	0.025	Grant et al. (1993a, b)

$D_{Ai,j,l,\mathrm{N,P}}$	decomposition rate of $A_{i,l,\mathrm{N,P}}$ by $M_{\boldsymbol{i,a,l,}\mathrm{C}}$	g N or P m^{-2} h^{-1}	[A7c]		
$D'_{Ai,j,l,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}	[A1a,A4c]		
$D_{Si,j,l,\mathrm{C}}$	decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ producing Q in [A13]	g C m^{-2} h^{-1}	[A1a,A7a,A31a]		
$\boldsymbol{D}_{Sj,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[$S_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	[A4a]	1.0, 1.0, 0.15, and 0.025 for *j* = protein, carbohydrate, cellulose, and lignin	Grant et al. (1993a, b)
$D_{Si,j,l,\mathrm{N,P}}$	decomposition rate of $S_{i,j,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m^{-2} h^{-1}	[A7a, A32]		
$D'_{Si,j,l,\mathrm{C}}$	specific decomposition rate of $S_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}	[A1a,A4a]		
$D_{Zi,j,l,\mathrm{C}}$	decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ producing Q in [A13]	g C m^{-2} h^{-1}	[A1b,A7b]		
$D_{Zi,j,\mathrm{N,P}}$	decomposition rate of $Z_{i,j,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$	g N or P m^{-2} h^{-1}	[A7b]		
$\boldsymbol{D}_{Zj,\mathrm{C}}$	specific decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[$Z_{i,l,\mathrm{C}}$]	g C g C^{-1} h^{-1}	[A4b]	0.25 and 0.05 for *j* = labile and resistant biomass	Grant et al. (1993a, b)
$D'_{Zi,j,l,\mathrm{C}}$	specific decomposition rate of $Z_{i,j,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C	g C g C^{-1} h^{-1}	[A1b,A4b]		
$\boldsymbol{\Delta G}$	energy yield of C oxidation and O_2 reduction	kJ g C^{-1}	[A21]	37.5	

$\boldsymbol{E}_{\mathbf{m}}$	energy requirement for growth of $M_{i,n,a,l}$	kJ g C^{-1}	[A21]	25	
$\boldsymbol{E}_{\boldsymbol{\Phi}}$	energy requirement for non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	g C g N^{-1}	[A28]	5	Waring and Running (1998)
$\boldsymbol{F}_{\mathbf{h}}$	fraction of products from microbial decomposition that are humified (function of clay content)		[A35]	0.167 + 0.167*clay	
$\boldsymbol{F}_{\mathbf{l}}$	fraction of microbial growth allocated to labile component $M_{i,n,l}$		[A25,A29,A30]	0.55	Grant et al. (1993a, b)
$\boldsymbol{F}_{\mathbf{r}}$	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 $Q_{i,l,\mathrm{C}}$ and $H_{i,l,\mathrm{C}}$		[A8]		
$f_{\mathrm{d}i,n,l\mathrm{N,P}}$	fraction of N or P released with $D_{Mi,n,j,l,\mathrm{C}}$ during decomposition	dimensionless	[A24]	0.33 $U_{\mathrm{NH4}} > 0$ 1.00 $U_{\mathrm{NH4}} < 0$ 0.33 $U_{\mathrm{PO4}} > 0$ 1.00 $U_{\mathrm{PO4}} < 0$	
$f_{\mathrm{tg}l}$	temperature function for microbial growth respiration	dimensionless	[A1,A6,A13, A23,A24]		
$f_{\mathrm{tm}l}$	temperature function for maintenance respiration	dimensionless	[A18,A19]		

$f_{\psi gl}$	soil water potential function for microbial, root or mycorrhizal growth respiration	dimensionless	[A13,A15]		Pirt (1975)
$\Phi_{i,n=f,j,l}$	non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	g N m^{-2} h^{-1}	[A27,A28,A29]		
$G_{i,l,\mathrm{C}}$	total C in substrate-microbe complex	g C Mg^{-1}	[A1,A2c,A3a,A8]		
$[H_2PO_4^-]$	concentration of $H_2PO_4^-$ in soil solution	g P m^{-3}	[A26]		
$\boldsymbol{H}_{\mathbf{a}}$	energy of activation	J mol^{-1}	[A6,C10]	65 x 10^3	Addiscott (1983)
$\boldsymbol{H}_{\mathbf{dh}}$	energy of high temperature deactivation	J mol^{-1}	[A6,C10]	225 x 10^3	
$\boldsymbol{H}_{\mathbf{dl}}$	energy of low temperature deactivation	J mol^{-1}	[A6,C10]	198 x 10^3	
$H_{Mi,n,j,l,\mathrm{C}}$	transfer of microbial C decomposition products to humus	g C m m^{-2} h^{-1}	[A35,A36]		
$H_{Mi,n,j,l,\mathrm{N,P}}$	transfer of microbial N or P decomposition products to humus	g N or P m^{-2} h^{-1}	[A36]		
$H_{Si,j,l,\mathrm{C}}$	transfer of C hydrolysis products to particulate OM	g C m^{-2} h^{-1}	[A31,A32,A33, A34]		
$H_{Si,j,l,\mathrm{N,P}}$	transfer of N or P hydrolysis products to particulate OM	g N or P m^{-2} h^{-1}	[A32,A34]		
$\boldsymbol{K}_{\boldsymbol{iS}}$	inhibition constant for microbial colonization of substrate	-	[A5]	0.5	Grant et al. (2010)
$\boldsymbol{K}_{\mathbf{NH_4}}$	M-M constant for NH_4^+ uptake at microbial surfaces	g N m^{-3}	[A26]	0.40	
$\boldsymbol{K}_{\mathbf{NO_3}}$	M-M constant for NO_3^- uptake at microbial surfaces	g N m^{-3}	[A26]	0.35	

$\boldsymbol{K_{\mathrm{PO_4}}}$	M-M constant for $H_2PO_4^-$ uptake at microbial surfaces	g P m^{-3}	[A26]	0.125	
$\boldsymbol{K_{\mathrm{i}D}}$	inhibition constant for $[M_{i,n,a}]$ on $S_{i,\mathrm{C}}$, $Z_{i,\mathrm{C}}$	g C m^{-3}	[A4]	25	Lizama and Suzuki (1990), Grant et al. (1993a, b)
$\boldsymbol{K_{\mathrm{m}D}}$	Michaelis–Menten constant for $D_{Si,j,\mathrm{C}}$	g C Mg^{-1}	[A4]	75	
$\boldsymbol{K_{\mathrm{m}Q_\mathrm{C}}}$	Michaelis–Menten constant for $R'_{\mathrm{h}i,n}$ on $[Q_{i,\mathrm{C}}]$	g C m^{-3}	[A13]	36	
$\boldsymbol{K_{\mathrm{O_2}}}$	Michaelis–Menten constant for reduction of O_{2s} by microbes, roots and mycorrhizae	g O_2 m^{-3}	[A17]	0.064	Griffin (1972)
$\boldsymbol{k_{\mathrm{ts}}}$	equilibrium rate constant for sorption	h^{-1}	[A8]	0.01	Grant et al. (1993a, b)
$\boldsymbol{L_{\mathrm{h}j}}$	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)
$\boldsymbol{M}$	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]		

$M_{i,n,j,l,\mathrm{C}}$	microbial C	g C m^{-2}	[A13,A17A23,A25,A26, A30,A36]	
$M_{i,n,j,l,\mathrm{N}}$	microbial N	g N m^{-2}	[A18,A27,A29]	
$M_{i,n,j,l,\mathrm{P}}$	microbial P	g P m^{-2}	[A24,A29,A26, A36]	
$M_{i,n,a,l,\mathrm{C}}$	active microbial C from heterotrophic population *n* associated with $G_{i,l,\mathrm{C}}$	g C m^{-2}	[A3,A13,A17, A30]	
$[M_{i,n,a,l,\mathrm{C}}]$	concentration of $M_{i,n,a}$ in soil water = $M_{i,n,a,l,\mathrm{C}} / \theta_l$	g C m^{-3}	[A3, A5]	
$[\mathrm{NH_4}^{+}{}_{i,n,j,l}]$	concentration of $\mathrm{NH_4^+}$ at microbial surfaces	g N m^{-3}	[A26]	
$[\mathbf{NH_4^{+}}_{\mathbf{mn}}]$	concentration of $\mathrm{NH_4^+}$ at microbial surfaces below which $U_{\mathrm{NH_4}} = 0$	g N m^{-3}	[A26]	0.0125
$[\mathrm{NO_3}^{-}{}_{i,n,j,l}]$	concentration of $\mathrm{NH_4^+}$ at microbial surfaces	g N m^{-3}	[A26]	
$[\mathbf{NO_3^{-}}_{\mathbf{mn}}]$	concentration of $\mathrm{NO_3^-}$ at microbial surfaces below which $U_{\mathrm{NO_3}} = 0$	g N m^{-3}	[A26]	0.03
$[\mathrm{H_2PO_4}^{-}{}_{i,n,j,l}]$	concentration of $\mathrm{H_2PO_4^-}$ at microbial surfaces	g N m^{-3}	[A26]	
$[\mathbf{H_2PO_4^{-}}_{\mathbf{mn}}]$	concentration of $\mathrm{H_2PO_4^-}$ at microbial surfaces below which $U_{\mathrm{PO_4}} = 0$	g N m^{-3}	[A26]	0.002

$[\mathrm{O}_{2\mathrm{m}i,n,l}]$	O_2 concentration at heterotrophic microsites	g O_2 m^{-3}	[A17]	
$[\mathrm{O}_{2\mathrm{s}l}]$	O_2 concentration in soil solution	g O_2 m^{-3}	[A17]	
$Q_{i,l,\mathrm{C}}$	*DOC* from products of $D_{Si,j,l,\mathrm{C}}$ [A3] and $D_{Zi,j,l,\mathrm{C}}$) [A5]	g C m^{-2}	[A8,A13,A22]	
$[Q_{i,l,\mathrm{C}}]$	solution concentration of $Q_{i,l,\mathrm{C}}$	g C Mg^{-1}	[A8,A13]	
$Q_{i,l,\mathrm{N,P}}$	*DON* and DOP from products of ($D_{Si,j,l,\mathrm{N,P}} + D_{Zi,j,l,\mathrm{N,P}}$)	g N or P m^{-2}	[A9,A22]	
$\boldsymbol{q_m}$	constant for reallocating $M_{i,a,l,\mathrm{C}}$ to $M_{i,d,l,\mathrm{C}}$	-	[A3a]	0.5
$\boldsymbol{R}$	gas constant	J mol^{-1} K^{-1}	[A6,A15,C10]	8.3143
$R_{\Phi i,n=f,j,l}$	respiration for non-symbiotic N_2 fixation by heterotrophic diazotrophs ($n = f$)	g C m^{-2} h^{-1}	[A28]	
$R_{\mathrm{g}i,n,l}$	growth respiration of $M_{i,n,a,l}$ on $Q_{i,l,\mathrm{C}}$ under nonlimiting O_2 and nutrients	g C g C^{-1} h^{-1}	[A20]	
R_h	total heterotrophic respiration of all $M_{i,n,a,l}$ under ambient DOC, O_2, nutrients, θ and temperature	g C m^{-2} h^{-1}	[A11]	
$R_{\mathrm{h}i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under ambient DOC, O_2, nutrients, θ and temperature	g C m^{-2} h^{-1}	[A5,A11,A14,A20, A21,A25]	
$\boldsymbol{R}_{\mathrm{h}i,n,l}$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2, DOC, θ and 25°C	g C g C^{-1} h^{-1}	[A12,A13]	

$\boldsymbol{R}_{\mathrm{h}}'{}_{n}$	specific heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting DOC, O_2, nutrients, θ and 25°C	g C g C^{-1} h^{-1}	[A12]	0.125	Shields et al. (1973)
$R_{\mathrm{h}}'{}_{i,n,l}$	heterotrophic respiration of $M_{i,n,a,l}$ under nonlimiting O_2 and ambient DOC, nutrients, θ and temperature	g C m^{-2} h^{-1}	[A13,A14,A16]		
$\boldsymbol{R}_{\mathrm{m}}$	specific maintenance respiration at 25°C	g C g N^{-1} h^{-1}	[A18]	0.0115	Barnes et al. (1998)
$R_{\mathrm{m}i,n,j,l}$	maintenance respiration by $M_{i,n,j,l}$	g C m^{-2} h^{-1}	[A18,A20,A21,A25]		
$r_{\mathrm{w}l}$	radius of r_{m} + water film at current water content	m	[A17]		
$\boldsymbol{r}_{\mathbf{m}}$	radius of heterotrophic microsite	m	[A17]	2.5×10^{-6}	
$r_{\mathrm{w}l}$	thickness of water films	m	[A17]		
$\boldsymbol{S}$	change in entropy	J mol^{-1} K^{-1}	[A6,C10]	710	Sharpe and DeMichelle (1977)
$[S_{i,j,l,\mathrm{C}}]$	concentration of $S_{i,j,l,\mathrm{C}}$ in soil	g C Mg^{-1}	[A4a]		
$S_{i,j,l,\mathrm{C}}$	mass of colonized litter, POC or humus C	g C m^{-2}	[A2a,A5,A7a,A33]		
$S'_{\boldsymbol{i,j,l,C}}$	mass of uncolonized litter, POC or humus C	g C m^{-2}	[A5]		

$S_{i,j,l,\mathrm{N,P}}$	mass of litter, POC or humus N or P	g N or P m^{-2}	[A7a,A33]	
T_{sl}	soil temperature	K	[A6,A15.A19]	
$U_{i,n,l\mathrm{C}}$	uptake of $Q_{i,l,\mathrm{C}}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g C m^{-2} h^{-1}	[A5,A21,A22,A25]	
$U_{i,n,\mathrm{N,P}}$	uptake of $Q_{i,l,\mathrm{N,P}}$ by $\Sigma_n M_{i,n,a,l}$ under limiting nutrient availability	g N or P m^{-2} h^{-1}	[A22,A29]	
$U_{\mathrm{NH4}i,n,j,l}$	NH_4^+ uptake by microbes	g N m^{-2} h^{-1}	[A26, A27,A29]	
$\boldsymbol{U'_{\mathrm{NH_4}}}$	maximum $U_{\mathrm{NH_4}}$ at 25 $^{\circ}$C and non-limiting NH_4^+	g N m^{-2} h^{-1}	[A26]	5.0×10^{-3}
$U_{\mathrm{NO3}i,n,j,l}$	NO_3^- uptake by microbes	g N m^{-2} h^{-1}	[A26,A27,A29]	
$\boldsymbol{U'_{\mathrm{NO_3}}}$	maximum $U_{\mathrm{NO_3}}$ at 25 $^{\circ}$C and non-limiting NO_3^-	g N m^{-2} h^{-1}	[A26]	5.0×10^{-3}
$U_{\mathrm{O2}i,n}$	O_2 uptake by $M_{i,n,a,l}$ under ambient O_2	g m^{-2} h^{-1}	[A14,A17]	
$U'_{\mathrm{O2}i,n}$	O_2 uptake by $M_{i,n,a,l}$ under nonlimiting O_2	g m^{-2} h^{-1}	[A14,A16,A17]	
$U_{\mathrm{PO4}i,n,j,l}$	$H_2PO_4^-$ uptake by microbes	g N m^{-2} h^{-1}	[A26,A27,A29]	
$\boldsymbol{U'_{\mathrm{PO_4}}}$	maximum $U_{\mathrm{PO_4}}$ at 25 $^{\circ}$C and non-limiting $H_2PO_4^-$	g N m^{-2} h^{-1}	[A26]	5.0×10^{-3}
$X_{i,l,\mathrm{C}}$	adsorbed C hydrolysis products	g C Mg^{-1}	[A8,A10]	
$X_{i,l,\mathrm{N,P}}$	adsorbed N or P hydrolysis products	g P Mg^{-1}	[A10]	
$\boldsymbol{y}$	selected to give a Q_{10} for f_{tm} of 2.25		[A19]	0.081

ψ_s	soil or residue water potential	MPa	[A15]
$Y_{i,l,\mathrm{C}}$	sorption of C hydrolysis products	g C $\mathrm{m}^{-2}\ \mathrm{h}^{-1}$	[A8,A9,A10]
$Y_{i,l,\mathrm{N,P}}$	sorption of N or P hydrolysis products	g P $\mathrm{m}^{-2}\ \mathrm{h}^{-1}$	[A9,A10]
$[Z_{i,j,l,\mathrm{C}}]$	concentration of $Z_{i,j,l,\mathrm{C}}$ in soil	g C Mg^{-1}	[A4b]
$Z_{i,j,l,\mathrm{C}}$	mass of microbial residue C in soil	g C m^{-2}	[A2b,A7b]
$Z_{i,j,l,\mathrm{N,P}}$	mass of microbial residue N or P in soil	g P m^{-2}	[A7b]

Appendix B: Soil-plant water relations

Canopy transpiration

$Rn_{\mathrm{c}i} + LE_{ci} + H_{\mathrm{c}i} + G_{\mathrm{c}i} = 0$	canopy energy balance	[B1a]
$\boldsymbol{L}E_{\mathrm{c}i} = L\ (e_{\mathrm{a}} - e_{\mathrm{c}i(T_{\mathrm{c}i},\psi_{ci})})/r_{\mathrm{a}i}$	LE from canopy evaporation	[B1b]
$\boldsymbol{L}E_{\mathrm{c}i} = L\ (e_{\mathrm{a}} - e_{\mathrm{c}i(T_{\mathrm{c}i},\psi_{ci})})/(r_{\mathrm{a}i} + r_{\mathrm{c}i})$ - $\boldsymbol{L}E_{\mathrm{c}i}$ from [B1b]	LE from canopy transpiration	[B1c]
$H_{\mathrm{c}i} = \rho C_{\mathrm{p}}(T_{\mathrm{a}} - T_{\mathrm{c}i})/r_{\mathrm{a}i}$	H from canopy energy balance	[B1d]
$r_{\mathrm{cmin}i} = 0.64\ (C_{\mathrm{b}} - \boldsymbol{C}_{\mathbf{i}}{}'_{\boldsymbol{i}})/\ V_{\mathrm{c}}{}'_{i}$	r_{c} driven by rates of carboxylation	[B2a]
$r_{\mathrm{c}i} = r_{\mathrm{cmin}i} + (\boldsymbol{r}_{\mathbf{cmax}\boldsymbol{i}} - r_{\mathrm{cmin}i})\ e^{(-\boldsymbol{\beta}\,\psi_{\mathrm{t}i})}$	*vs*. diffusion	[B2b]
	r_{c} constrained by water status	

$r_{ai} = \{(\ln((z_u - z_{di})/z_{ri})^2 /(\boldsymbol{K}^2 u_a)\}/(1 - 10\,Ri)$	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]
$\psi_{ti} = \psi_{ci} - \psi_{\pi i}$		[B4]

Root and mycorrhizal water uptake

$U_{wi} = \Sigma_l\,\Sigma_r\,U_{wi,r,l}$		[B5]
$U_{wi,r,l} = (\psi_c'_i - \psi_s'_l)/(\Omega_{si,r,l} + \Omega_{ri,r,l} + \Sigma_x\,\Omega_{ai,r,l,x})$	U_w along hydraulic gradient	[B6]
$\psi_c'_i = \psi_{ci} + 0.01\,z_{bi}$		[B7]
$\psi_s'_l = \psi_{sl} - 0.01\,z_l$		[B8]
$\Omega_{si,r,l} = \ln\{(d_{i,r,l}/r_{i,r,l})/(2\pi\,L_{i,r,l}\,\kappa_{ri,r,l})\}\;\theta_{wl}/\theta_{pl}$		[B9]
$\Omega_{ri,r,l} = \boldsymbol{\Omega'}_{\mathbf{ri,r}}/L_{i,r,l}$		[B10]
$\Omega_{ai,r,l,x=1} = \boldsymbol{\Omega'}_{\mathbf{ai,r}}\,z_l /\{n_{i,r,l,1}\,(r_{i,r,l,1}/\mathbf{r'}_{i,r})^4\} + \boldsymbol{\gamma\Omega'}_{\mathbf{ai,r}}\,z_{bi} /\{n_{i,r,l,1}\,(r_{bi}/r_b'_i)^4\}\Sigma_{i,r,l}\,(M_{i,r,l})\,/M_{i,r,l}$		[B11]
$\Omega_{ai,r,l,x=2} = \boldsymbol{\Omega}_{\mathbf{ai,r}}\,(L_{i,r,l,2}/n_{i,r,l,2})\,/\{n_{i,r,l,2}\,(r_{i,r,l,2}/r'_{i,r})^4\}$		[B12]
$\delta L_{i,r,l,1}/\delta t = \delta M_{i,r,l,1}/\delta t\;\nu_r\;/\{\rho_r\,(1 - \theta_{Pi,r})\,(\pi\,r_{i,r,l,1}^2)\}$		[B13]

Canopy water potential

$(e_{\mathrm{a}} - e_{i(T_{\mathrm{c}i})})/(r_{\mathrm{a}i} + r_{\mathrm{c}i})$ [B1] $= \Sigma_l \Sigma_{\mathrm{r}}(\psi_{\mathrm{c}}'_i - \psi_{\mathrm{s}}'_l)/(\Omega_{\mathrm{s}i,r,l} + \Omega_{\mathrm{r}i,r,l} + \Sigma_x \Omega_{\mathrm{a}i,r,l,x}) + X_{\mathrm{c}i}\delta\psi_{\mathrm{c}i}/\delta t$	ψ_{c} solved when transpiration from [B1-B4] (LHS) equals uptake from [B5-B13] + change in storage (RHS)	[B14]

Definition of variables in appendix B

Variable	Definition	Unit	Equation	Value	Reference
	Subscripts				
I	plant species or functional type: coniferous, deciduous, annual, perennial, C_3, C_4, monocot, dicot etc.				
J	branch or tiller				
K	Node				
L	soil or canopy layer				
M	leaf azimuth				
n	leaf inclination				
o	leaf exposure (sunlit *vs*. shaded)				
r	root or mycorrhizae				
	Variables				

$\boldsymbol{\beta}$	stomatal resistance shape parameter	MPa^{-1}	[B2b,C4,C9]	-5.0	Grant and Flanagan (2007)
C_b	[CO_2] in canopy air	$\mu mol\ mol^{-1}$	[B2,C2,C5]		
$\boldsymbol{C_i{}'_i}$	[CO_2] in canopy leaves at ψ_{ci} = 0 MPa	$\mu mol\ mol^{-1}$	[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]		
$G_{\boldsymbol{ci}}$	canopy storage heat flux	$W\ m^{-2}$	[B1]		
$H_{\boldsymbol{ci}}$	canopy sensible heat flux	$W\ m^{-2}$	[B1]		
K	von Karman’s constant		[B3a]	0.41	
$\kappa_{ri,r,l}$	hydraulic conductivity between soil and root surface	$m^2\ MPa^{-1}\ h^{-1}$	[B9]		
$\boldsymbol{\gamma}$	scaling factor for bole axial resistance from primary root axial resistance	-	[B11]	1.6 x 10^4	Grant et al. (2007)
$\boldsymbol{L}$	latent heat of evaporation	$J\ g^{-1}$	[B1]	2460	
$\boldsymbol{LE_{ci}}$	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]		
$\boldsymbol{\Omega}_{\mathbf{ai,r}}$	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)
$\Omega_{\mathrm{ai},r,l,x}$	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]		
$\boldsymbol{\Omega}_{\mathbf{ri,r}}$	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)
$\Omega_{\mathrm{ri},r,l}$	radial resistance to water transport from surface to axis of roots or mycorrhizae	MPa h m^{-1}	[B6,B10]		
$\Omega_{\mathrm{si},r,l}$	radial resistance to water transport from soil to surface of roots or mycorrhizae	MPa h m^{-1}	[B6,B9]		
$\theta_{\mathrm{w}l}$	soil water content	m^3 m^{-3}	[B9]		
$\theta_{\mathrm{p}l}$	soil porosity	m^3 m^{-3}	[B9]		

$\theta_{\mathrm{P}i,r}$	root porosity	m^3 m^{-3}	[B13]		
Ri	Richarson number		[B3a,B3b]		van Bavel and Hillel (1976)
$Rn_{\mathrm{c}i}$	canopy net radiation	W m^{-2}	[B1]		
$r_{\mathrm{a}i}$	aerodynamic resistance to vapor flux from canopy	s m^{-1}	[B1,B3a]		
$r_{\mathrm{b}i}$	radius of bole at ambient $\psi_{\mathrm{c}i}$	m	[B11]		
$r_{\mathrm{b}}'{}_{i}$	radius of bole at $\psi_{\mathrm{c}i} = 0$ MPa	m	[B11]		
$r_{\mathrm{c}i}$	canopy stomatal resistance to vapor flux	s m^{-1}	[B1,B2b]		
$\boldsymbol{r_{\mathrm{cmax}i}}$	canopy cuticular resistance to vapor flux	s m^{-1}	[B2b]	5.0 x 10^3	Larcher (2001)
$r_{\mathrm{cmin}i}$	minimum $r_{\mathrm{c}i}$ at $\psi_{\mathrm{c}i} = 0$ MPa	s m^{-1}	[B2,B2b]		
$r_{i,r,l,x}$	radius of primary (x=1) or secondary (x=2) roots or mycorrhizae at ambient $\psi_{\mathrm{r}i\,l,z}$	m	[B9,B11,B12,B13]		
$\boldsymbol{r'}_{i,r}$	radius of secondary roots or mycorrhizae at $\psi_{\mathrm{r}i\,l,z} = 0$ 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 (1998a)

T_a	air temperature	K	[B3b]		
T_c	canopy temperature	K	[B3b]		
$U_{\mathrm{w}i}$	total water uptake from all rooted soil layers	$\mathrm{m^3\ m^{-2}\ h^{-1}}$	[B5,B14]		
$U_{\mathrm{w}i,r,l}$	water uptake by root and mycorrhizal surfaces in each soil layer	$\mathrm{m^3\ m^{-2}\ h^{-1}}$	[B5,B6]		
u_a	wind speed measured at z_u	$\mathrm{m\ s^{-1}}$	[B3a,B3b]		
$V_\mathrm{c}'_i$	potential canopy CO_2 fixation rate at $\psi_{\mathrm{c}i} = 0$ MPa	$\mu\mathrm{mol\ m^{-2}\ s^{-1}}$	[B2]		
ν_r	root specific volume	$\mathrm{m^3\ g\ FW^{-1}}$	[B13]	10^{-6}	Grant (1998a)
X_{ci}	canopy capacitance	$\mathrm{m^3\ m^{-2}\ MPa^{-1}}$	[B14]		
$\psi_{\mathrm{c}i}$	canopy water potential	MPa	[B4,B7,B14]		
$\psi_\mathrm{c}'_i$	$\psi_{\mathrm{c}i}$ + canopy gravitational potential	MPa	[B6,B7]		
$\psi_{\pi i}$	canopy osmotic potential	MPa	[B4]		
ψ_{sl}	soil water potential	MPa	[B8]		
$\psi_\mathrm{s}'_l$	ψ_{sl} + soil gravitational potential	MPa	[B6,B8]		
$\psi_{\mathrm{t}i}$	canopy turgor potential	MPa	[B2b,B4]	1.25 at $\psi_\mathrm{c} = 0$	
$z_{\mathrm{b}i}$	length of bole from soil surface to top of canopy	m	[B7,B11]		
$z_{\mathrm{d}i}$	canopy zero-plane displacement height	m	[B3a]		Perrier (1982)
z_l	depth of soil layer below surface	m	[B8,B11]		

z_{r}	canopy surface roughness	m	[B3a,B3b]	Perrier (1982)
z_{u}	height of wind speed measurement	m	[B3a,B3b]	

Appendix C: Gross primary productivity and autotrophic respiration

C$_3$ gross primary productivity

$GPP = \Sigma_{i,j,k,l,m,n,o}\,(V_{\mathrm{c}i,j,k,l,m,n,o} = V_{\mathrm{g}i,j,k,l,m,n,o})\,A_{i,j,k,l,m,n,o}$	solve for $C_{\mathrm{i}i,j,k,l,m,n,o}$ at which $V_{\mathrm{c}i,j,k,l,m,n,o} = V_{\mathrm{g}i,j,k,l,m,n,o}$	[C1]
$V_{\mathrm{g}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - C_{\mathrm{i}i,j,k,l,m,n,o})/r_{\mathrm{l}i,j,k,l,m,n,o}$	diffusion	[C2]
$V_{\mathrm{c}i,j,k,l,m,n,o} = min\{V_{\mathrm{b}i,j,k,l,m,n,o}, V_{\mathrm{j}i,j,k,l,m,n,o}\}$	carboxylation	[C3]
$r_{\mathrm{l}i,j,k,l,m,n,o} = r_{\mathrm{lmin}i,j,k,l,m,n,o} + (r_{\mathrm{lmax}i} - r_{\mathrm{lmin}i,j,k,l,m,n,o})\,e^{(-\boldsymbol{\beta}\psi_{\mathrm{t}i})}$	r_{l} is leaf-level equivalent of r_{c}	[C4]
$r_{\mathrm{lmin}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - \boldsymbol{C}_{\mathbf{i}}'_{\boldsymbol{i}})/\,V_{\mathrm{c}}'_{i,j,k,l,m,n,o}$	minimum r_{l} is driven by carboxylation	[C5]

$V_{\mathrm{b}i,j,k,l,m,n,o} = V_{\mathrm{bmax}i,j,k}(C_{\mathrm{c}i,j,k,l,m,n,o} - \mathit{\Gamma}_{i,j,k})/(C_{\mathrm{c}i,j,k,l,m,n,o}) + K_{\mathrm{c}_i})\, f_{\psi\ i,j,k,l,m,n,o}\ f_{\mathrm{iC}\boldsymbol{i}}$ CO$_2$, water, temperature and nutrient constraints on V_{b} [C6a]

$V_{\mathrm{bmax}_{i,j,k}} = \boldsymbol{V}_{\mathbf{b}}{}'_{i}\, \boldsymbol{F}_{\mathbf{rubisco}_i}\, M_{i,j,k,prot} / A_{i,j,k}\ f_{\mathrm{tb}\boldsymbol{i}}$ [C6b]

$\mathit{\Gamma}_{i,j,k} = 0.5\ O_{\mathrm{c}}\ V_{\mathrm{omax}_{i,j,k}}\ \boldsymbol{K}_{\mathbf{c}_i} / (V_{\mathrm{bmax}_{i,j,k}}\ \boldsymbol{K}_{\mathbf{o}_i})$ [C6c]

$V_{\mathrm{omax}_{i,j,k}} = \boldsymbol{V}_{\mathbf{o}}{}'_{i}\, \boldsymbol{F}_{\mathbf{rubisco}_i}\, M_{i,j,k,prot} / A_{i,j,k}\ f_{\mathrm{to}\boldsymbol{i}}$ [C6d]

$K_{\mathrm{c}_i} = \boldsymbol{K}_{\mathbf{c}_i}\, f_{\mathrm{tkc}i}\ (1 + O_{\mathrm{c}}/\ (\boldsymbol{K}_{\mathbf{o}_i}\, f_{\mathrm{tko}i}))$ [C6e]

$V_{\mathrm{j}i,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o}\ Y_{i,j,k,l,m,n,o}\ f_{\psi\ i,j,k,l,m,n,o}\ f_{\mathrm{iC}\boldsymbol{i}}$ [C7]

$J_{i,j,k,l,m,n,o} = (\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k} - ((\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k})^{2} - 4\boldsymbol{\alpha\varepsilon}\, I_{i,l,m,n,o}\, J_{\mathrm{max}i,j,k})^{0.5})/(2\boldsymbol{\alpha})$ water, temperature and nutrient constraints on V_{j} [C8a]

$J_{\mathrm{max}i,j,k} = \boldsymbol{V}_{\mathbf{j}}{}'_{i}\, \boldsymbol{F}_{\mathbf{chlorophyll}_i}\, M_{i,j,k,prot} / A_{i,j,k}\ f_{\mathrm{tj}i}$ [C8b]

$f_{\psi\ i,j,k,l,m,n,o} = (r_{\mathrm{lmin}_{i,j,k,l,m,n,o}} / r_{\mathrm{l}_{i,j,k,l,m,n,o}})^{0.5}$ non-stomatal effect related to stomatal effect [C9]

$$f_{\mathrm{tb}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\}$$

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

$$f_{\mathrm{to}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{o}} - \boldsymbol{H}_{\mathbf{ao}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]]$$

[C10b]

temperature sensitivity of $\boldsymbol{K}_{\mathbf{c}_i}$, $\boldsymbol{K}_{\mathbf{o}_i}$

$$f_{\mathrm{tj}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{j}} - \boldsymbol{H}_{\mathbf{aj}}/(\boldsymbol{R}T_{\mathrm{c}i})]/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\}$$

[C10c]

$$f_{\mathrm{tkc}i} = \exp[\boldsymbol{B}_{\mathbf{kc}} - \boldsymbol{H}_{\mathbf{akc}}/(\boldsymbol{R}T_{\mathrm{c}i})]$$

[C10d]

$$f_{\mathrm{tko}i} = \exp[\boldsymbol{B}_{\mathbf{ko}} - \boldsymbol{H}_{\mathbf{ako}}/(\boldsymbol{R}T_{\mathrm{c}i})]$$

[C10e]

$$f_{\mathrm{iC}\boldsymbol{i}} = min\{\sigma_{\mathrm{N}i,j}/\boldsymbol{(}\sigma_{\mathrm{N}i,j} + \sigma_{\mathrm{C}i,j}/\boldsymbol{K}_{\mathbf{iC_N}}), \sigma_{\mathrm{P}i,j}/\boldsymbol{(}\sigma_{\mathrm{P}i,j} + \sigma_{\mathrm{C}i,j}/\boldsymbol{K}_{\mathbf{iC_P}})\}$$

product inhibition of V_{b}, V_{j} from σ_{N} and σ_{P} *vs.* σ_{C} in shoots [C11]

$$\delta M_{\mathrm{L}_{\mathrm{R}i,j,k}}/\delta t = \delta M_{\mathrm{L}_{i,j,k}}/\delta t \min\{[\boldsymbol{N'}_{\mathbf{leaf}} + (\boldsymbol{N}_{\mathbf{leaf}} - \boldsymbol{N'}_{\mathbf{leaf}})\, f_{\mathrm{iC}\boldsymbol{i}}]/\mathbf{N}_{\mathbf{prot},}\ [\boldsymbol{P'}_{\mathbf{leaf}} + (\boldsymbol{P}_{\mathbf{leaf}} - \boldsymbol{P'}_{\mathbf{leaf}})\, f_{\mathrm{iC}\boldsymbol{i}}]/\mathrm{P}_{\mathrm{prot}}\}$$

leaf structural protein growth [C12]

Autotrophic respiration

$$R_{\mathrm{a}} = \Sigma_i \Sigma_{,j} (R_{\mathrm{c}i,j} + R_{\mathrm{s}i,j}) + \Sigma_i \Sigma_l \Sigma_z (R_{\mathrm{c}i,r,l} + R_{\mathrm{s}i,r,l}) + \boldsymbol{E}_{\mathbf{N,P}} (U_{\mathrm{NH4}i,r,l} + U_{\mathrm{NO3}i,r,l} + U_{\mathrm{PO4}i,r,l})$$

total autotrophic respiration [C13]

$$R_{\mathrm{c}i,j} = \boldsymbol{R}_{\mathrm{c}}'\sigma_{\mathrm{C}i,j}\; f_{\mathrm{ta}i} \tag{C14a}$$

O$_2$ constraint on root respiration from active uptake coupled with diffusion of O$_2$ from soil as for heterotrophic respiration in [A17], and from active uptake coupled with diffusion of O$_2$ from roots

$$R_{\mathrm{c}i,r,l} = \boldsymbol{R}_{\mathrm{c}}'\sigma_{\mathrm{C}\,i,r,l}\; f_{\mathrm{ta}\,i,l}\; (U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l}) \tag{C14b}$$

$$U_{\mathrm{O2}i,r,l} = U'_{\mathrm{O2}\,i,r,l}\; [\mathrm{O}_{2\mathrm{r}i,r,l}]/([\mathrm{O}_{2\mathrm{r}i,r,l}] + \boldsymbol{K}_{\mathbf{O_2}}) \tag{C14c}$$

$$\begin{aligned} &= U_{\mathrm{w}_{i,r,l}}[\mathrm{O}_{2\mathrm{s}l}] + 2\pi L_{i,r,l}\, D_{\mathrm{sO2}}\,([\mathrm{O}_{2\mathrm{s}l}] - [\mathrm{O}_{2\mathrm{r}i,r,l}])\,\ln\{(r_{\mathrm{s}l} + r_{\mathrm{r}i,r,l})/\, r_{\mathrm{r}i,r,l}\} \\ &\quad + 2\pi L_{i,r,l}\, D_{\mathrm{rO2}}\,([\mathrm{O}_{2\mathrm{q}i,r,l}] - [\mathrm{O}_{2\,\mathrm{r}i,r,l}])\,\ln(r_{\mathrm{q}i,r,l})/\, r_{\mathrm{r}i,r,l}) \end{aligned} \tag{C14d}$$

$$U'_{\mathrm{O2}\,i,r,l} = 2.67\, R_{\mathrm{a}}'{}_{i,r,l} \tag{C14e}$$

$$R_{\mathrm{s}i,j} = -\,min\{0.0, R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j}\} \tag{C15}$$

remobilization when $R_{\mathrm{m}} > R_{\mathrm{c}}$

$$R_{\mathrm{m}i,j} = \Sigma_z\, (\mathrm{N}_{i,j,z}\, \boldsymbol{R}_{\mathbf{m}}'\; f_{\mathrm{tm}i}) \tag{C16}$$

maintenance respiration

$$R_{\mathrm{g}i,j} = max\{0.0, min\{(R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j})\, min\{1.0, max\{0.0, \psi_{\mathrm{t}i} - \psi_{\mathrm{t}}'\}\} \tag{C17}$$

growth when $R_{\mathrm{m}} < R_{\mathrm{c}}$

Growth and senescence

$$l_{i,j,z,\mathrm{C}} = R_{\mathrm{s}i,j}\, M_{\mathrm{L_N}i,j} / M_{\mathrm{L_R}i,j} \tag{C18}$$

senescence drives litterfall of non-remobilizable material

$$l_{i,j,z,\mathrm{N}} = l_{i,j,z,\mathrm{C}}\,\mathbf{N_{prot}}\,(1.0 - \boldsymbol{X}_{\mathbf{mx}}\,f_{\mathrm{xN}i,j}) \qquad \text{[C19a]}$$

$$l_{i,j,z,\mathrm{P}} = l_{i,j,z,\mathrm{C}}\,\mathbf{P_{prot}}\,(1.0 - \boldsymbol{X}_{\mathbf{mx}}\,f_{\mathrm{xP}i,j}) \qquad \text{[C19b]}$$

$$f_{\mathrm{xN}i,j} = \sigma_{\mathrm{C}i,j}/(\sigma_{\mathrm{C}i,j} + \sigma_{\mathrm{N}i,j}/\boldsymbol{K}_{\mathbf{xN}}) \qquad \text{[C19c]}$$

$$f_{\mathrm{xP}i,j} = \sigma_{\mathrm{C}i,j}/(\sigma_{\mathrm{C}i,j} + \sigma_{\mathrm{P}i,j}\,/\boldsymbol{K}_{\mathbf{xP}}) \qquad \text{[C19d]}$$

litterfall of N and P is driven by that of C but reduced by translocation to to σ_{N} and σ_{P} according to ratios of σ_{N} and σ_{P} with σ_{C}

$$\delta M_{\mathrm{B}i,j}/\delta t = \Sigma_z\,[R_{\mathrm{g}i,j}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,z})/\boldsymbol{Y}_{\mathbf{g}i,z}] - R_{\mathrm{s}i,j} - l_{i,j,\mathrm{C}} \qquad \text{[C20a]}$$

branch growth driven by R_{g}

$$\delta M_{\mathrm{R}i,r,l}/\delta t = [R_{\mathrm{g}i,r,l}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,r})/\boldsymbol{Y}_{\mathbf{g}i,r}] - R_{\mathrm{s}i,r,l} - l_{i,r,l,\mathrm{C}} \qquad \text{[C20b]}$$

root growth driven by R_{g}

$$\delta A_{\mathrm{L}i,j,k,l}/\delta t = \boldsymbol{\chi}\,(M_{\mathrm{L}i,j,k,l}\,/y_i)^{-0.33}\,\delta M_{\mathrm{L}i,j,k,l}/\delta t\ \min\{1, \max\{0, \psi_{ti} - \psi_{t}'\}\} \qquad \text{[C21a]}$$

leaf expansion driven by leaf mass growth

$$\delta L_{i,r,l,1}/\delta \mathrm{t} = (\delta M_{\mathrm{R}i,r,l,1}\,/\delta \mathrm{t})/y_i\,\nu_r\,/\{\boldsymbol{\rho}_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r}\,)\,(\pi\,r_{\mathrm{r}i,r,l,1}{}^2)\} \qquad \text{[C21b]}$$

$$\delta L_{i,r,l,2}/\delta \mathrm{t} = (\delta M_{\mathrm{R}i,r,l,2}\,/\delta \mathrm{t})\,\nu_r\,/\{\boldsymbol{\rho}_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r}\,)\,(\pi\,r_{\mathrm{r}i,r,l,2}{}^2)\} \qquad \text{[C21c]}$$

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

$$f_{\mathrm{ta}i} = T_{\mathrm{c}i}\{\exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}}/(\boldsymbol{R}T_{\mathrm{c}i})]\}/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\}$$

Arrhenius function for R_a [C22a]

$$f_{\mathrm{tm}i} = e^{(0.0811*(T_{ci} - 298.15))}$$

temperature function for R_m [C22b]

Root and mycorrhizal nutrient uptake

$$U_{\mathrm{NH4}i,r,l} = \{U_{\mathrm{w}i,r,l}[\mathrm{NH_4}^+{}_l] + 2\pi L_{i,r,l}D_{\mathrm{eNH4}l}\ ([\mathrm{NH_4}^+{}_l] - [\mathrm{NH_4}^+{}_{i,r,l}])\ /\ \ln(d_{i,r,l}\ /r_{\mathrm{r}i,r,l})\}$$ [C23a]

$$= \boldsymbol{U'}_{\mathbf{NH_4}}\ (U_{\mathrm{O2}i,r,l}\ /U'_{\mathrm{O2}i,r,l})\ A_{i,r,l}\ ([\mathrm{NH_4}^+{}_{i,r,l}] - [\mathbf{NH_4}^{\mathbf{+}}{}_{\mathbf{mn}}])/([\mathrm{NH_4}^+{}_{i,r,l}] - [\mathbf{NH_4}^{\mathbf{+}}{}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\ f_{\mathrm{t}il}\, f_{\mathrm{iN}\boldsymbol{i,r,l}}$$ [C23b]

$$U_{\mathrm{NO3}i,r,l} = \{U_{\mathrm{w}i,r,l}\ [\mathrm{NO_3}^-{}_l] + 2\pi L_{i,r,l}\ D_{\mathrm{eNO3}l}\ ([\mathrm{NO_3}^-{}_l] - [\mathrm{NO_3}^-{}_{i,r,l}])\ /\ \ln(d_{i,r,l}\ /r_{\mathrm{r}i,r,l})\}$$ [C23c]

$$= \boldsymbol{U'}_{\mathbf{NO_3}}\ (U_{\mathrm{O2}i,r,l}\ /U'_{\mathrm{O2}i,r,l})\ A_{i,r,l}\ ([\mathrm{NO_3}^-{}_{i,r,l}] - [\mathbf{NO_3}^{\mathbf{-}}{}_{\mathbf{mn}}]\ )/([\mathrm{NO_3}^-{}_{i,r,l}] - [\mathbf{NO_3}^{\mathbf{-}}{}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\ f_{\mathrm{t}il}\ f_{\mathrm{iN}\boldsymbol{i,r,l}}$$ [C23d]

$$U_{\mathrm{PO4}i,r,l} = \{U_{\mathrm{w}i,r,l}\ [\mathrm{H_2PO_4}^-{}_l] + 2\pi L_{i,r,l}D_{\mathrm{ePO4}l}\ ([\mathrm{H_2PO_4}^-{}_l] - [\mathrm{H_2PO_4}^-{}_{i,r,l}])\ /\ \ln(d_{i,r,l}\ /r_{\mathrm{r}i,r,l})\}$$

$$= \boldsymbol{U'}_{\mathbf{PO_4}}\ (U_{\mathrm{O2}i,r,l}\ /U'_{\mathrm{O2}i,r,l})\ A_{i,r,l}\ ([\mathrm{H_2PO_4}^-{}_{i,r,l}] - [\mathbf{H_2PO_4}^{\mathbf{-}}{}_{\mathbf{mn}}])/([\mathrm{H_2PO_4}^-{}_{i,r,l}] - [\mathbf{H_2PO_4}^{\mathbf{-}}{}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{PO_4}})\ f_{\mathrm{tg}l}\ f_{\mathrm{iP}\boldsymbol{i,r,l}}$$ [C23e]

$$f_{\mathrm{iN}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{N}i,r,l}/\boldsymbol{K}_{\mathbf{iN_C}})$$ [C23f]

$$f_{\mathrm{iP}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{P}i,r,l}/\boldsymbol{K}_{\mathbf{iP_C}})$$ [C23g]

[C23h]

root N and P uptake from mass flow + diffusion coupled with active uptake of $\mathrm{NH_4}^+$, $\mathrm{NO_3}^-$ and $\mathrm{H_2PO_4}^-$ constrained by $\mathrm{O_2}$ uptake, as for microbial N and P uptake in [A26]

product inhibition of U_{NH4}, U_{NO3} and U_{PO4} determined by σ_N and σ_P *vs.* σ_C in roots

$\mathrm{C_4}$ gross primary productivity

$\mathrm{C_4}$ mesophyll

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

[C24]

$$V_{\mathrm{g(m4)}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - C_{\mathrm{i(m4)}i,j,k,l,m,n,o})/r_{\mathrm{lf}i,j,k,l,m,n,o}$$

gaseous diffusion [C25]

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

mesophyll carboxylation [C26]

$$r_{\mathrm{lf}i,j,k,l,m,n,o} = r_{\mathrm{lfmin}i,j,k,l,m,n,o} + (r_{\mathrm{lfmax}i} - r_{\mathrm{lfmin}i,j,k,l,m,n,o})\, e^{(-\beta\, \psi_{\mathrm{t}i})}$$

[C27]

$$r_{\mathrm{lfmin}i,j,k,l,m,n,o} = (C_{\mathrm{b}} - C_{\mathrm{i(m4)}}{'}_{i})/\, V_{\mathrm{c}_0\mathrm{(m4)}i,j,k,l,m,n,o}$$

[C28]

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

CO_2-limited carboxylation [C29]

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

light-limited carboxylation [C30]

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

irradiance response function [C31]

$$V_{\mathrm{bmax(m4)}i,j,k} = V_{\mathrm{bmax(m4)}}{'}\, [N_{\mathrm{pep(m4)}i,j,k}]'\ N_{\mathrm{lf}i,j,k}\ A_{\mathrm{lf}i,j,k}\ f_{\mathrm{C(m4)}i,j,k}\, f_{\psi i}\ f_{\mathrm{tv}i}$$

PEPc activity [C32]

$$J_{\mathrm{max(m4)}i,j,k} = J_{\mathrm{max}}{'}\, [N_{\mathrm{chl(m4)}i,j,k}\ ]'\ N_{\mathrm{lf}i,j,k}\ A_{\mathrm{lf}i,j,k}\ f_{\mathrm{C(m4)}i,j,k},\, f_{\psi i}\ f_{\mathrm{tv}i}$$

chlorophyll activity [C33]

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

C_4 product inhibition [C34]

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

non-stomatal water limitation [C35]

$$f_{\mathrm{tv}i} = T_{\mathrm{c}i}\{\exp[B - H_{\mathrm{a}}/(RT_{\mathrm{c}i})]\}/\{1 + \exp[(H_{\mathrm{dl}} - ST_{\mathrm{c}i})/(RT_{\mathrm{c}i})] + \exp[(ST_{\mathrm{c}i} - H_{\mathrm{dh}})/(RT_{\mathrm{c}i})]\}$$

temperature limitation [C36]

C_4 mesophyll-bundle sheath exchange

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

mesophyll-bundle sheath transfer [C37]

$$V_{\chi\mathrm{C4(b4)}i,j,k} = \kappa_{\chi\mathrm{C4(b4)}}\, \chi_{\mathrm{C4(b4)}i,j,k} /(1.0 + C_{\mathrm{c(b4)}i,j,k} / K_{\mathrm{I}\chi_{\mathrm{C4(b4)}}})$$

bundle sheath decarboxylation [C38]

$$V_{\phi\mathrm{(b4)}i,j,k} = \kappa_{\mathrm{Cc(b4)}}\, (C_{\mathrm{c(b4)}i,j,k} - C_{\mathrm{c(m4)}i,j,k})\, (12 \text{ x } 10^{-9})\, W_{\mathrm{lf(b4)}i,j,k}$$

bundle sheath-mesophyll leakage [C39]

$\delta\chi_{\mathrm{C4(m4)}i,j,k} /\delta t = \Sigma_{l,m,n,o}\ V_{\mathrm{c(m4)}i,j,k,l,m,n,o} - V_{\chi\mathrm{C4(m4)}i,j,k}$ mesophyll carboxylation products [C40]

$\delta\chi_{\mathrm{C4(b4)}i,j,k}/\delta t = V_{\chi\mathrm{C4(m4)}i,j,k} - V_{\chi\mathrm{C4(b4)}i,j,k}$ bundle sheath carboxylation products [C41]

$\delta C_{\mathrm{c(b4)}i,j,k}/\delta t = V_{\chi\mathrm{C4(b4)}i,j,k} - V_{\phi\mathrm{(b4)}i,j,k} - \Sigma_{l,m,n,o}\ V_{\mathrm{c(b4)}i,j,k,l,m,n,o}$ bundle sheath CO_2 concentration [C42]

C_4 bundle sheath

$V_{\mathrm{c(b4)}i,j,k,l,m,n,o} = min\{V_{\mathrm{b(b4)}i,j,k}, V_{\mathrm{j(b4)}i,j,k,l,m,n,o}\}$ bundle sheath carboxylation [C43]

$V_{\mathrm{b(b4)}i,j,k} = V_{\mathrm{bmax(b4)}i,j,k}(C_{\mathrm{c(b4)}i,j,k} - \Gamma_{\mathrm{(b4)}i,j,k})/(C_{\mathrm{c(b4)}i,j,k}) + K_{\mathrm{c(b4)}_i})$ CO_2-limited carboxylation [C44]

$V_{\mathrm{j(b4)}i,j,k,l,m,n,o} = J_{\mathrm{(b4)}i,j,k,l,m,n,o}\ Y_{\mathrm{(b4)}i,j,k}$ light- limited carboxylation [C45]

$J_{\mathrm{(b4)}i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(b4)}i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(b4)}i,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\mathrm{max(b4)}i,j,k})^{0.5})/(2\alpha)$ irradiance response function [C46]

$V_{\mathrm{bmax(b4)}i,j,k} = V_{\mathrm{bmax(b4)}}'\,[N_{\mathrm{rub(b4)}i,j,k}]'\ N_{\mathrm{lf}i,j,k}\ A_{\mathrm{lf}i,j,k}\ f_{\mathrm{C(c3)}i,j,k}\ f_{\psi i}\ f_{\mathrm{tv}i}$ RuBPc activity [C47]

$J_{\mathrm{max(b4)}i,j,k} = J_{\mathrm{max}}'\,[N_{\mathrm{chl(b4)}i,j,k}]'\ N_{\mathrm{lf}i,j,k}\ A_{\mathrm{lf}i,j,k}\ f_{\mathrm{C(c3)}i,j,k}\ f_{\psi i}\ f_{\mathrm{tv}i}$ chlorophyll activity [C48]

$f_{\mathrm{C(c3)}i,j,k} = \min\{[\nu_{\mathrm{lf}i,j}]/([\nu_{\mathrm{lf}i,j}]+ [\chi_{\mathrm{c3(b4)}i,j}]/K_{\mathrm{I}\nu_{\mathrm{lf}}}), [\pi_{\mathrm{lf}i,j}]/([\pi_{\mathrm{lf}i,j}]+ [\chi_{\mathrm{c3(b4)}i,j}]/K_{\mathrm{I}\pi_{\mathrm{lf}}})\}$ C_3 product inhibition [C49]

Definition of variables in appendix C

Variable	Definition	Unit	Equation	Value	Reference
		Subscripts			

i	species or functional type: evergreen, coniferous, deciduous, annual, perennial, C_3, C_4, monocot, dicot, legume etc.
j	branch or tiller
k	Node
l	soil or canopy layer
m	leaf azimuth
n	leaf inclination
o	leaf exposure (sunlit *vs*. shaded)
z	organ including leaf, stem, root, mycorrhizae

Variables

A	leaf, root or mycorrhizalsurface area	m^2 m^{-2}	[C1,C6b,C6d,C8b, C21,C23,C32,C33 ,C47]		
$\boldsymbol{\beta}$	shape parameter for stomatal effects on CO_2 diffusion and non-stomatal effects on carboxylation	MPa^{-1}	[C4 C27,C35,]	-5.0	Grant and Flanagan (2007)

B	parameter such that $f_{\mathrm{t}} = 1.0$ at $T_c = 298.15$ K		[C36]	17.533	
$\boldsymbol{B}_{\mathbf{j}}$	parameter such that $f_{\mathrm{tj}\boldsymbol{i}} = 1.0$ at $T_{\mathrm{c}} = 298.15$ K		[C10c]	17.363	
$\boldsymbol{B}_{\mathbf{kc}}$	parameter such that $f_{\mathrm{tkc}i} = 1.0$ at $T_{\mathrm{c}} = 298.15$ K		[C10d]	22.187	
$\boldsymbol{B}_{\mathbf{ko}}$	parameter such that $f_{\mathrm{tko}i} = 1.0$ at $T_{\mathrm{c}} = 298.15$ K		[C10e]	8.067	
$\boldsymbol{B}_{\mathbf{o}}$	parameter such that $f_{\mathrm{to}\boldsymbol{i}} = 1.0$ at $T_{\mathrm{c}} = 298.15$ K		[C10b]	24.221	
$\boldsymbol{B}_{\mathbf{v}}$	parameter such that $f_{\mathrm{tv}\boldsymbol{i}} = 1.0$ at $T_{\mathrm{c}} = 298.15$ K		[C10a, C22]	26.238	
C_{b}	[CO_2] in canopy air	μmol mol^{-1}	[C2,C5 C25,C28]		
$C_{\mathrm{c(b4)}}$	[CO_2] in C_4 bundle sheath	μM	[C38,C39,C42,C44]		
$C_{\mathrm{c(m4)}}$	[CO_2] in C_4 mesophyll in equilibrium with $C_{\mathrm{i}i,j,k,l,m,n,o}$	μM	[C29,C39]		
C_{c}	[CO_2] in canopy chloroplasts in equilibrium with $C_{\mathrm{i}i,j,k,l,m,n,o}$	μM	[C6]		
$C_{\mathrm{i(m4)}}'$	[CO_2] in C_4 mesophyll air when $\psi_{\mathrm{c}i} = 0$	μmol mol^{-1}	[C28]	0.45 x C_{b}	
$C_{\mathrm{i(m4)}}$	[CO_2] in C_4 mesophyll air	μmol mol^{-1}	[C25]		
$\mathrm{C}_{i,j,z=l}$	C content of leaf ($z = l$)	g C m^{-2}	[C18]		
$\boldsymbol{C}_{\mathbf{i}}'$	[CO_2] in canopy leaves when $\psi_{\mathrm{c}i} = 0$	μmol mol^{-1}	[C5]	0.70 x C_{b}	Larcher (2001)
C_{i}	[CO_2] in canopy leaves	μmol mol^{-1}	[C2]		

$D_{\mathrm{e\ NH}_{4}l}$	effective dispersivity-diffusivity of NH_4^+ during root uptake	$m^2\ h^{-1}$	[C23]		
$D_{\mathrm{e\ NO}_{3}l}$	effective dispersivity-diffusivity of NO_3^- during root uptake	$m^2\ h^{-1}$	[C23]		
$D_{\mathrm{e\ PO}_{4}l}$	effective dispersivity-diffusivity of $H_2PO_4^-$ 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]	$(\pi\ L_{s,z}\ /\Delta \mathrm{z})^{-1/2}$	Grant (1998a)
$\boldsymbol{E}_{\mathbf{N,P}}$	energy cost of nutrient uptake	g C g N^{-1} or P^{-1}	[C13]	2.15	Veen (1981)
$f_{\mathrm{C(c3)}}$	C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll	–	[C47,C48,C49]		
$f_{\mathrm{C(m4)}}$	C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	–	[C32,C33,C34]		
$\boldsymbol{F}_{\mathbf{chl}}$	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]		
$\boldsymbol{F}_{\mathbf{rubisco}}$	fraction of leaf protein in rubisco	-	[C6b,d]	0.125	
f_{ta}	temperature effect on $R_{\mathrm{a}i,j}$	–	[C14, C22]		
f_{tb}	temperature effect on carboxylation	–	[C6b,C10a]		
f_{tg}	temperature function for root or mycorrhizal growth respiration	dimensionless	[C23]		
f_{tj}	temperature effect on electron transport		[C8b,C10c]		
f_{tkc}	temperature effect on $\boldsymbol{K}_{\mathbf{c}_i}$		[C6e,C10d]		Bernacchi et al. (2001, 2003)
f_{tko}	temperature effect on $\boldsymbol{K}_{\mathbf{o}_i}$		[C6e,C10e]		Bernacchi et al. (2001, 2003)
f_{tm}	temperature effect on $R_{\mathrm{m}i,j}$	–	[C16, C22b]	$Q_{10} = 2.25$	
f_{to}	temperature effect on oxygenation		[C6d,C10b]		
f_{tv}	temperature effect on carboxylation	–	[C32,C33,C36,C47,C48]		

f_{xN}	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ N translocated out of leaf or root during senescence	–	[C19a,c]		
f_{xP}	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ P translocated out of leaf or root during senescence	–	[C19b,d]		
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–	[C6a,C7,C9]		Medrano et al. (2002)
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–	[C32,C33,C35C47,C48]		
H_{a}	energy of activation	J mol^{-1}	[C36]	57.5 x 10^{3}	
$\boldsymbol{H}_{\mathbf{aj}}$	energy of activation for electron transport	J mol^{-1}	[C10c]	43 x 10^{3}	Bernacchi et al. (2001, 2003)
$\boldsymbol{H}_{\mathbf{akc}}$	parameter for temperature sensitivity of $\boldsymbol{K}_{\mathbf{c}_i}$	J mol^{-1}	[C10d]	55 x 10^{3}	Bernacchi et al. (2001, 2003)
$\boldsymbol{H}_{\mathbf{ako}}$	parameter for temperature sensitivity of $\boldsymbol{K}_{\mathbf{o}_i}$	J mol^{-1}	[C10e]	20 x 10^{3}	Bernacchi et al. (2001, 2003)
$\boldsymbol{H}_{\mathbf{ao}}$	energy of activation for oxygenation	J mol^{-1}	[C10b, C22]	60 x 10^{3}	Bernacchi et al. (2001, 2003)

$\boldsymbol{H}_{\mathbf{av}}$	energy of activation for carboxylation	J mol^{-1}	[C10a, C22]	65 x 10^3	Bernacchi et al. (2001, 2003)
$\boldsymbol{H}_{\mathbf{dh}}$	energy of high temperature deactivation	J mol^{-1}	[C10, C22]	222.5 x 10^3	
H_{dh}	energy of high temperature deactivation	J mol^{-1}	[C36]	220 x 10^3	
$\boldsymbol{H}_{\mathbf{dl}}$	energy of low temperature deactivation	J mol^{-1}	[C10, C22]	198.0 x 10^3	
H_{dl}	energy of low temperature deactivation	J mol^{-1}	[C36]	190 x 10^3	
I	Irradiance	μmol m^{-2} s^{-1}	[C8a,]		
$J_{(\mathrm{b4})}$	electron transport rate in C_4 bundle sheath	μmol m^{-2} s^{-1}	[C45,C46]		
$J_{(\mathrm{m4})}$	electron transport rate in C_4 mesophyll	μmol m^{-2} s^{-1}	[C30,C31]		
J	electron transport rate in C_3 mesophyll	μmol m^{-2} s^{-1}	[C7,C8a]		
J_{max}'	specific electron transport rate at non-limiting I and 25°C when $\psi_{ci} = 0$ and nutrients are nonlimiting	μmol g^{-1} s^{-1}	[C33,C48]	400	
$J_{\mathrm{max(b4)}}$	electron transport rate in C_4 bundle sheath at non-limiting I	μmol m^{-2} s^{-1}	[C46,C48]		
$J_{\mathrm{max(m4)}}$	electron transport rate in C_4 mesophyll at non-limiting I	μmol m^{-2} s^{-1}	[C31,C33]		
J_{max}	electron transport rate at non-limiting I, $\psi_{\mathrm{c}i}$, temperature and N,P	μmol m^{-2} 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)
$\boldsymbol{K_{c}}$	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]		
$\boldsymbol{K_{iC_N}}$	inhibition constant for growth in shoots from σ_C *vs.* σ_N	$g\ C\ g\ N^{-1}$	[C11]	100	Grant (1998a)
$\boldsymbol{K_{iC_P}}$	inhibition constant for growth in shoots from σ_C *vs.* σ_P	$g\ C\ g\ P^{-1}$	[C11]	1000	Grant (1998a)
$K_{I\chi C4(b4)}$	constant for CO_2 product inhibition of C_4 decarboxylation in C_4 bundle sheath	µM	[C38]	1000.0	
$K_{I\chi C4(m4)}$	constant for C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	µM	[C34]	5×10^6	

$K_{\mathrm{I}\nu_{\mathrm{lf}}}$	constant for C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll caused by $[\nu_{\mathrm{lf}i,j}]$	g C g N^{-1}	[C49]	100	
$K_{\mathrm{I}\pi_{\mathrm{lf}}}$	constant for C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll caused by $[\pi_{\mathrm{lf}i,j}]$	g C g P^{-1}	[C49]	1000	
$\boldsymbol{K}_{\mathbf{iN_C}}$	inhibition constant for N uptake in roots from $\sigma_{\mathrm{C}i,j}$ *vs.* $\sigma_{\mathrm{N}j}$	g N g C^{-1}	[C23]	0.1	Grant (1998a)
$\boldsymbol{K}_{\mathbf{iP_C}}$	inhibition constant for P uptake in roots from $\sigma_{\mathrm{C}i,j}$ *vs.* $\sigma_{\mathrm{P}i,j}$ roots	g P g C^{-1}	[C23]	0.01	Grant (1998a)
$\boldsymbol{K}_{\mathbf{NH_4}}$	M-M constant for NH_4^+ uptake at root or mycorrhizal surfaces	g N m^{-3}	[C23]	0.40	Barber and Silberbush (1984)
$\boldsymbol{K}_{\mathbf{NO_3}}$	M-M constant for NO_3^- uptake at root or mycorrhizal surfaces	g N m^{-3}	[C23]	0.35	Barber and Silberbush (1984)
$\boldsymbol{K}_{\mathbf{PO_4}}$	M-M constant for $H_2PO_4^-$ uptake root or mycorrhizal surfaces	g P m^{-3}	[C23]	0.125	Barber and Silberbush (1984)
$\boldsymbol{K}_{\mathbf{O_2}}$	Michaelis-Menten constant for root or mycorrhizal O_2 uptake	g m^{-3}	[C14c]	0.064	Griffin (1972)

$\boldsymbol{K_o}$	inhibition constant for O_2 in carboxylation	μM	[C6c,C6e]	500 at 25 ^oC	Farquhar et al. (1980)
$\boldsymbol{K_{xN}}$	inhibition constant for remobilization of leaf or root N during senescence	g N g C^{-1}	[C19c]	0.1	
$\boldsymbol{K_{xP}}$	inhibition constant for remobilization of leaf or root P during senescence	g P g C^{-1}	[C19d]	0.01	
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]		
M_L	leaf C phytomass	g C m^{-2}	[C12,C21]		
M_{L_N}, M_{L_R}	non-remobilizable, remobilizable leaf C phytomass	g C m^{-2}	[C12,C18]		
M_R	root C phytomass	g C m^{-2}	[C20,C21]		
M_{iprot}	leaf protein phytomass calculated from leaf N, P contents	g N m^{-2}	[C6b,C6d,C8b,C12]		
N,P	N or P content of organ z	g N m^{-2}	[C16, C19]		
$\mathbf{N_{prot}}$	N content of protein remobilized from leaf or root	g N C^{-1}	[C12,C19a]	0.4	

$[\mathrm{NH_4}^{+}{}_{i,r,l}]$	concentration of $\mathrm{NH_4}^{+}$ at root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{NH_4}^{+}{}_{\mathbf{mn}}]$	concentration of $\mathrm{NH_4}^{+}$ at root or mycorrizal surfaces below which $U_{\mathrm{NH_4}} = 0$	g N m^{-3}	[C23]	0.0125	Barber and Silberbush (1984)
$[\mathrm{NO_3}^{-}{}_{i,r,l}]$	concentration of $\mathrm{NH_4}^{+}$ at root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{NO_3}^{-}{}_{\mathbf{mn}}]$	concentration of $\mathrm{NO_3}^{-}$ at root or mycorrizal surfaces below which $U_{\mathrm{NO_3}} = 0$	g N m^{-3}	[C23]	0.03	Barber and Silberbush (1984)
$[\mathrm{H_2PO_4}^{-}{}_{i,r,l}]$	concentration of $\mathrm{H_2PO_4}^{-}$ root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{H_2PO_4}^{-}{}_{\mathbf{mn}}]$	concentration of $\mathrm{H_2PO_4}^{-}$ at root or mycorrizal surfaces below which $U_{\mathrm{PO_4}} = 0$	g N m^{-3}	[C23]	0.002	Barber and Silberbush (1984)
$\boldsymbol{N}_{\mathbf{leaf}}$	maximum leaf structural N content	g N g C^{-1}	[C12]	0.10	
$\boldsymbol{N'}_{\mathbf{leaf}}$	minimum leaf structural N content	g N g C^{-1}	[C12]	0.33 x $\boldsymbol{N}_{\mathbf{leaf}}$	
N_{lf}	total leaf N	g N m^{-2} leaf	[C32,C33,C47,C48]		
$[N_{\mathrm{chl(b4)}}]'$	ratio of chlorophyll N in $\mathrm{C_4}$ bundle sheath to total leaf N	g N g N^{-1}	[C48]	0.05	
$[N_{\mathrm{chl(m4)}}]'$	ratio of chlorophyll N in $\mathrm{C_4}$ mesophyll to total leaf N	g N g N^{-1}	[C33]	0.05	
$[N_{\mathrm{pep(m4)}}]'$	ratio of PEP carboxylase N in $\mathrm{C_4}$ mesophyll to total leaf N	g N g N^{-1}	[C32]	0.025	

$[N_{\mathrm{rub(b4)}}]'$	ratio of RuBP carboxylase N in C_4 bundle sheath to total leaf N	g N g N^{-1}	[C47]	0.025
O_{2q}	aqueous O_2 concentration in root or mycorrhizal aerenchyma	g m^{-3}	[C14c,d]	
O_{2r}	aqueous O_2 concentration at root or mycorrhizal surfaces	g m^{-3}	[C14c,d]	
O_{2s}	aqueous O_2 concentration in soil solution	g m^{-3}	[C14c,d]	
O_c	[O_2] in canopy chloroplasts in equilibrium with $O_{2\ \mathrm{in}}$ atm.	μM	[C6c,C6e]	
$\boldsymbol{P}_{\mathbf{leaf}}$	maximum leaf structural P content	g P g C^{-1}	[C12]	0.10
$\boldsymbol{P'}_{\mathbf{leaf}}$	minimum leaf structural P content	g P g C^{-1}	[C12]	0.33 x $\boldsymbol{P}_{\mathbf{leaf}}$
$\mathbf{P}_{\mathbf{prot}}$	P content of protein remobilized from leaf or root	g P C^{-1}	[C12,C19b]	0.04
$[\pi_{\mathrm{lf}}]$	concentration of nonstructural root P uptake product in leaf	g P g C^{-1}	[C49]	
$\boldsymbol{\theta}_{\mathbf{P}}$	root or mycorrhizal porosity	m^3 m^{-3}	[C21b]	0.1 – 0.5
$\boldsymbol{R}$	gas constant	J mol^{-1} K^{-1}	[C10, C22]	8.3143
R	gas constant	J mol^{-1} K^{-1}	[C36]	8.3143
R_a	total autotrophic respiration	g C m^{-2} h^{-1}	[C13]	
R_a'	R_a under nonlimiting O_2	g C m^{-2} h^{-1}	[C14]	

$\boldsymbol{R}_{\mathrm{c}}'$	specific autotrophic respiration of $\sigma_{\mathrm{C}i,j}$ at $T_{ci} = 25\ ^{\mathrm{o}}\mathrm{C}$	g C g C^{-1} h^{-1}	[C14]	0.015	
R_{c}	autotrophic respiration of $\sigma_{\mathrm{C}i,j}$ or $\sigma_{\mathrm{C}i,r,l}$	g C m^{-2} h^{-1}	[C13,C14,C17, C15]		
R_{g}	growth respiration	g C m^{-2} h^{-1}	[C17,C20]		
r_{lf}	leaf stomatal resistance	s m^{-1}	[C25,C27,C39]		
$r_{\mathrm{lfmax}i}$	leaf cuticular resistance	s m^{-1}	[C27]		
$r_{\mathrm{lfmin}i,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{\mathrm{c}i} = 0$	s m^{-1}	[C27,C28,C35		
$r_{\mathrm{l}i,j,k,l,m,n,o}$	leaf stomatal resistance	s m^{-1}	[C2,C4,C9]		
$r_{\mathrm{lmax}i}$	leaf cuticular resistance	s m^{-1}	[C4]		
$r_{\mathrm{lmin}i,j,k,l,m,n,o}$	leaf stomatal resistance when $\psi_{\mathrm{c}i} = 0$	s m^{-1}	[C4,C5,C9]		
$\boldsymbol{R}_{\mathbf{m}}'$	specific maintenance respiration of $\sigma_{\mathrm{C}i,j}$ at $T_{ci} = 25\ ^{\mathrm{o}}\mathrm{C}$	g C g N^{-1} h^{-1}	[C16]	0.0115	Barnes et al. (1998)
$R_{\mathrm{m}i,j}$	above-ground maintenance respiration	g C m^{-2} h^{-1}	[C16,C17,C15]		
$r_{\mathrm{q}i,r,l}$	radius of root aerenchyma	m	[C14d]		
$r_{\mathrm{r}i,r,l}$	root or mycorrhizal radius	m	[C14d,C21b,c,C23a,c,e]	1.0×10^{-4} or 5.0×10^{-6}	

$R_{si,j}$	respiration from remobilization of leaf C	g C m^{-2} h^{-1}	[C13,C15,C18, C20]		
r_{sl}	thickness of soil water films	m	[C14d]		
ρ_r	dry matter content of root biomass	g g^{-1}	[C21b]	0.125	
$\boldsymbol{S}$	change in entropy	J mol^{-1} K^{-1}	[C10, C22]	710	Sharpe and DeMichelle (1977)
S	change in entropy	J mol^{-1} K^{-1}	[C36]	710	
σ_{C}	nonstructural C product of CO_2 fixation	g C g C^{-1}	[C11, C19c,d, C23g,h]		
σ_{N}	nonstructural N product of root uptake	g N g C^{-1}	[C11, C19c, C23g,h]		
σ_{P}	nonstructural P product of root uptake	g P g C^{-1}	[C11, C19d, C23g,h]		
T_{c}	canopy temperature	K	[C10, C22]		
T_{c}	canopy temperature	^{o}C	[C36]		
$U_{\mathrm{NH4}i,r,l}$	NH_4^+ uptake by roots or mycorrhizae	g N m^{-2} h^{-1}	[C23]		

$\boldsymbol{U'_{\mathrm{NH_4}}}$	maximum $U_{\mathrm{NH_4}}$ at 25 $^{\mathrm{o}}$C and non-limiting $\mathrm{NH_4^+}$	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush (1984)
$U_{\mathrm{NO3}i,r,l}$	$\mathrm{NO_3^-}$ uptake by roots or mycorrhizae	g N m^{-2} h^{-1}	[C23]		
$\boldsymbol{U'_{\mathrm{NO_3}}}$	maximum $U_{\mathrm{NO_3}}$ at 25 $^{\mathrm{o}}$C and non-limiting $\mathrm{NO_3^-}$	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush (1984)
$U_{\mathrm{PO4}i,r,l}$	$\mathrm{H_2PO_4^-}$ uptake by roots or mycorrhizae	g N m^{-2} h^{-1}	[C23]		
$\boldsymbol{U'_{\mathrm{PO_4}}}$	maximum $U_{\mathrm{PO_4}}$ at 25 $^{\mathrm{o}}$C and non-limiting $\mathrm{H_2PO_4^-}$	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush (1984)
$U_{\mathrm{O2}i,r,l}$	$\mathrm{O_2}$ uptake by roots and mycorrhizae under ambient $\mathrm{O_2}$	g O m^{-2} h^{-1}	[C14b,c,C23b,d,f]		
$U'_{\mathrm{O2}i,l.r}$	$\mathrm{O_2}$ uptake by roots and mycorrhizae under nonlimiting $\mathrm{O_2}$	g O m^{-2} h^{-1}	[C14b,c,C23b,d,f]		
$U_{\mathrm{w}i,r,l}$	root water uptake	m^3 m^{-2} h^{-1}	[C14d,C23]		
$V_{\phi(\mathrm{b4})i,j,k}$	$\mathrm{CO_2}$ leakage from $\mathrm{C_4}$ bundle sheath to $\mathrm{C_4}$ mesophyll	g C m^{-2} h^{-1}	[C39,C42]		
$\boldsymbol{V_{\mathrm{b}}'}$	specific rubisco carboxylation at 25 $^{\mathrm{o}}$C	µmol g $^{-1}$ rubisco s^{-1}	[C6b]	45	Farquhar et al. (1980)
$V_{\mathrm{b(b4)}i,j,k}$	$\mathrm{CO_2}$-limited carboxylation rate in $\mathrm{C_4}$ bundle sheath	µmol m^{-2} s^{-1}	[C43,C44]		
$V_{\mathrm{b(m4)}i,j,k,l,m,n,o}$	$\mathrm{CO_2}$-limited carboxylation rate in $\mathrm{C_4}$ mesophyll	µmol m^{-2} s^{-1}	[C26]		
$V_{\mathrm{b}i,j,k,l,m,n,o}$	$\mathrm{CO_2}$-limited leaf carboxylation rate	µmol m^{-2} s^{-1}	[C3,C6]		

$V_{\mathrm{bmax(b4)}}'$	RuBP carboxylase specific activity in C_4 bundle sheath at 25°C when $\psi_{\mathrm{c}i} = 0$ and nutrients are nonlimiting	μmol g^{-1} s^{-1}	[C47]	75
$V_{\mathrm{bmax(b4)}i,j,k}$	CO_2-nonlimited carboxylation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}	[C44,C47]	
$V_{\mathrm{bmax(m4)}}'$	PEP carboxylase specific activity in C_4 mesophyll at 25°C when $\psi_{\mathrm{c}i} = 0$ and nutrients are nonlimiting	μmol g^{-1} s^{-1}	[C32]	150
$V_{\mathrm{bmax(m4)}i,j,k}$	CO_2-nonlimited carboxylation rate in C_4 mesophyll	μmol m^{-2} s^{-1}	[C29,C32]	
$V_{\mathrm{bmax}i,j,k}$	leaf carboxylation rate at non-limiting CO_2, $\psi_{\mathrm{c}i}$, T_{c} and N,P	μmol m^{-2} s^{-1}	[C6a,C6b,C6c]	
$V_{\mathrm{c(b4)}i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}	[C43]	
$V_{\mathrm{c(m4)}i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 mesophyll	μmol m^{-2} s^{-1}	[C24,C26,C40,C41]	
$V_{\mathrm{c0(m4)}\,i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 mesophyll when $\psi_{\mathrm{c}i} = 0$ MPa	μmol m^{-2} s^{-1}	[C28]	
$V_{\mathrm{c}i,j,k,l,m,n,o}$	leaf CO_2 fixation rate	μmol m^{-2} s^{-1}	[C1,C3]	
$V_{\mathrm{c}}'_{i,j,k,l,m,n,o}$	leaf CO_2 fixation rate when $\psi_{\mathrm{c}i} = 0$	μmol m^{-2} s^{-1}	[C5]	
$V_{\mathrm{g(m4)}i,j,k,l,m,n,o}$	CO_2 diffusion rate into C_4 mesophyll	μmol m^{-2} s^{-1}	[C24,C25]	
$V_{\mathrm{g}i,j,k,l,m,n,o}$	leaf CO_2 diffusion rate	μmol m^{-2} s^{-1}	[C1,C2]	

$\boldsymbol{V}_{\mathbf{j}}'$	specific chlorophyll e$^-$ transfer at 25 $^{\mathrm{o}}$C	μmol g $^{-1}$ chlorophyll s^{-1}	[C8b]	450	Farquhar et al. (1980)
$V_{\mathrm{j(b4)}i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C_4 bundle sheath	μmol m^{-2} s^{-1}	[C43,C45]		
$V_{\mathrm{j(m4)}i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C_4 mesophyll	μmol m^{-2} s^{-1}	[C26,C30]		
$V_{\mathrm{j}i,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	μmol m^{-2} s^{-1}	[C3,C7]		
$\boldsymbol{V}_{\mathbf{o}}'$	specific rubisco oxygenation at 25 $^{\mathrm{o}}$C	μmol g $^{-1}$ rubisco s^{-1}	[C6d]	9.5	Farquhar et al. (1980)
$V_{\mathrm{omax}i,j,k}$	leaf oxygenation rate at non-limiting O_2, $\psi_{\mathrm{c}i}$, T_{c} and N,P	μmol m^{-2} s^{-1}	[C6c,d]		
$V_{\chi\mathrm{C4(b4)}i,j,k}$	decarboxylation of C_4 fixation product in C_4 bundle sheath	g C m^{-2} h^{-1}	[C38,C41,C42]		
$V_{\chi\mathrm{C4(m4)}}$	transfer of C_4 fixation product between C_4 mesophyll and bundle sheath	g C m^{-2} h^{-1}	[C37]		
$[\nu_{\mathrm{lf}}]$	concentration of nonstructural root N uptake product in leaf	g N g C^{-1}	[C49]		
ν_r	specific volume of root biomass	m^3 g^{-1}	[C21b]		
$W_{\mathrm{lf(b4)}}$	C_4 bundle sheath water content	g m^{-2}	[C37,C39]		
$W_{\mathrm{lf(m4)}}$	C_4 mesophyll water content	g m^{-2}	[C37]		

χ_{mx}	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	[C19a,b]	0.6	Kimmins (2004)
$Y_{(\mathrm{b4})}$	carboxylation yield from electron transport in C_4 bundle sheath	μmol CO_2 μmol e^{-1}	[C45]		
$Y_{(\mathrm{m4})}$	carboxylation yield from electron transport in C_4 mesophyll	μmol CO_2 μmol e^{-1}	[C30]		
$\boldsymbol{Y}_{\mathbf{g}}$	fraction of $\sigma_{\mathrm{C}i,j}$ used for growth expended as $R_{\mathrm{g}i,j,z}$ 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]		
Y	carboxylation yield	μmol CO_2 μmol e^{-1}	[C7]		
Γ	CO_2 compensation point	μM	[C6a,C6c]		
$\Gamma_{(\mathrm{b4})}$	CO_2 compensation point in C_4 bundle sheath	μM	[C44]		
$\Gamma_{(\mathrm{m4})}$	CO_2 compensation point in C_4 mesophyll	μM	[C29]		

$\boldsymbol{\alpha}$	shape parameter for response of J to I	-	[C8a]	0.7	
α	shape parameter for response of J to I	-	[C31,C46]	0.75	
$\boldsymbol{\chi}$	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]		
$\boldsymbol{\varepsilon}$	quantum yield	μmol e^{-} μmol quanta^{-1}	[C8a]	0.45	Farquhar et al. (1980)
ε	quantum yield	μmol e^{-} μmol quanta^{-1}	[C31,C46]	0.45	Farquhar et al. (1980)
$\kappa_{Cc(b4)}$	conductance to CO_2 leakage from C_4 bundle sheath	h^{-1}	[C39]	20	
ψ_t	canopy turgor potential	MPa	[C4]	1.25 at $\psi_c = 0$	

Appendix D: Soil water, heat, gas and solute fluxes

Surface water flux

$Q_{\mathrm{r}x(x,y)} = v_{x(x,y)}d_{\mathrm{m}x,y}L_{y(x,y)}$	2D Manning equation in *x* (EW)	[D1]
$Q_{\mathrm{r}y(x,y)} = v_{y(x,y)}d_{\mathrm{m}x,y}L_{x(x,y)}$	and *y* (NS) directions	
$d_{x,y} = \max(0,d_{\mathrm{w}(x,y)} + d_{\mathrm{i}(x,y)} - d_{\mathrm{s}(x,y)})d_{\mathrm{w}(x,y)}/(d_{\mathrm{w}(x,y)} + d_{\mathrm{i}(x,y)})$	surface water depth	[D2]
$v_{x(x,y)} = R^{0.67}s_{x(x,y)}{}^{0.5}/z_{\mathrm{r}(x,y)}$	runoff velocity over E slope	[D3]
$v_{y(x,y)} = R^{0.67}s_{y(x,y)}{}^{0.5}/z_{\mathrm{r}(x,y)}$	runoff velocity over S slope	
$v_{x(x,y)} = -R^{0.67}s_{x(x,y)}{}^{0.5}/z_{\mathrm{r}(x,y)}$	runoff velocity over W slope	
$v_{y(x,y)} = -R^{0.67}s_{y(x,y)}{}^{0.5}/z_{\mathrm{r}(x,y)}$	runoff velocity over N slope	
$\Delta(d_{\mathrm{w}(x,y)}A_{x,y})/\Delta t = Q_{\mathrm{r},x(x,y)} - Q_{\mathrm{r},x+1(x,y)} + Q_{\mathrm{r},y(x,y)} - Q_{\mathrm{r},y+1(x,y)} + \mathrm{P} - \mathrm{E}_{x,y} - Q_{\mathrm{wz}(x,y,1)}$	2D kinematic wave theory for	[D4]
	overland flow	
$R = s_{\mathrm{r}}d_{\mathrm{m}}/[2(s_{\mathrm{r}}{}^2 + 1)0.5]$	wetted perimeter	[D5a]
$s_{x(x,y)} = 2abs[(Z + d_{\mathrm{s}} + d_{\mathrm{m}})_{x,y} - (Z + d_{\mathrm{s}} + d_{\mathrm{m}})_{x+1,y}]/(L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and	
	pooled surface water in *x* (EW)	[D5b]
$s_{y(x,y)} = 2abs[(Z + d_{\mathrm{s}} + d_{\mathrm{m}})_{x,y} - (Z + d_{\mathrm{s}} + d_{\mathrm{m}})_{x,y+1}]/(L_{y(x,y)} + L_{y(x,y+1)})$	and *y* (NS) directions	

$\boldsymbol{L}E_{\mathrm{l}} = L\,(e_{\mathrm{a}} - e_{\mathrm{l}(T_l,\psi_l)})/r_{\mathrm{a}l}$	evaporation from surface litter	[D6a]
$\boldsymbol{L}E_{\mathrm{s}} = L\,(e_{\mathrm{a}} - e_{\mathrm{s}(T_s,\psi_s)})/r_{\mathrm{a}s}$	evaporation from soil surface	[D6b]

Subsurface water flux

$Q_{\mathrm{w}x(x,y,z)} = K'_x(\psi_{\mathrm{s}x,y,z} - \psi_{\mathrm{s}x+1,y,z})$	3D Richard’s or Green-Ampt equation depending on saturation of source or target cell in *x* (EW), *y* (NS) and *z* (vertical) directions	[D7]
$Q_{\mathrm{w}y(x,y,z)} = K'_y(\psi_{\mathrm{s}x,y,z} - \psi_{\mathrm{s}x,y+1,z})$		
$Q_{\mathrm{w}z(x,y,z)} = K'_z(\psi_{\mathrm{s}x,y,z} - \psi_{\mathrm{s}x,y,z+1})$		
$\Delta\theta_{w\,x,y,z}/\Delta t = (Q_{\mathrm{w}x(x,y)} - Q_{\mathrm{w}x+1(x,y)} + Q_{\mathrm{w}y(x,y)} - Q_{\mathrm{w}y+1(x,y)} + Q_{\mathrm{w}z(x,y)} - Q_{\mathrm{w}z+1(x,y)} + Q_{f(x,y,z)})/\,L_{z(x,y,z)}$	3D water transfer plus freeze-thaw	[D8]
$K'_x = 2K_{x,y,z}K_{x+1,y,z}/(K_{x,y,z}\,L_{x,(x+1,y,z)} + K_{x+1,y,z}\,L_{x,(x,y,z)})$	in direction *x* if source and destination cells are unsaturated	[D9a]
$= 2K_{x,y,z}/(L_{x(x+1,y,z)} + L_{x(x,y,z)})$	in direction *x* if source cell is saturated	[D9b]
$= 2K_{x+1,y,z}/(L_{x(x+1,y,z)} + L_{x(x,y,z)})$	in direction *x* if destination cell is saturated	
$K'_y = 2K_{x,y,z}K_{x,y+1,z}/(K_{x,y,z}\,L_{y(x,y+1,z)} + K_{x,y+1,z}\,L_{y(x,y,z)})$	in direction *y* if source and destination cells are unsaturated	[D9a]

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

Exchange with water table

$Qmat_{tx(x,y,z)} = Kmat_{x,y,z}\ [\psi' - \psi_{sx,y,z} + 0.01(d_{zx,y,z} - WTD_x)]/(L_{tx} + 0.5\ L_{x,(x,y,z)})$	if $d_{zx,y,z} < WTD_x$ then $\psi_{sx,y,z} > \psi' + 0.01(d_{zx,y,z} - WTD_x)$ for all depths z from $d_{zx,y,z}$ to WTD_x	[D10]
$Qmat_{tx(x,y,z)} = Kmat_{x,y,z}\ [\psi' - \psi_{sx,y,z} + 0.01(d_{zx,y,z} - WTD_x)]/(L_{tx} + 0.5\ L_{x,(x,y,z)})$	or if $d_{zx,y,z} > WTD_x$ then $\psi_{sx,y,z} > 0.01(WTD_x - d_{zx,y,z}) - \psi'$ for all depths z from WTD_x to $d_{zx,y,z}$	

$Qmac_{\mathrm{t}x(x,y,z)} = Kmac_{x,y,z}\ [0.01*\min(0,\ d_{\mathrm{z}x,y,z} - L_{z(x,y,z)}*(\min(1, \max(0,\ \theta_{mac}))\text{-}0.5)\ \text{-}\ WTD_x)]/(L_{\mathrm{t}x} + 0.5\ L_{x,(x,y,z)})$	if $d_{\mathrm{z}x,y,z} < WTD_x$ then $\psi_{\mathrm{s}x,y,z} > \psi' + 0.01(d_{\mathrm{z}x,y,z} - WTD_x)$ for all depths z from $d_{\mathrm{z}x,y,z}$ to WTD_x	[D10a]
$Qmac_{\mathrm{t}x(x,y,z)} = Kmac_{x,y,z}\ [0.01*\max(0,\ d_{\mathrm{z}x,y,z} - L_{z(x,y,z)}*(\min(1, \max(0,\ \theta_{mac}))\text{-}0.5)\ \text{-}\ WTD_x)]/(L_{\mathrm{t}x} + 0.5\ L_{x,(x,y,z)})$	or if $d_{\mathrm{z}x,y,z} > WTD_x$ then $\psi_{\mathrm{s}x,y,z} > 0.01(WTD_x\ \text{-}\ d_{\mathrm{z}x,y,z})\ \text{-}\ \psi'$ for all depths z from WTD_x to $d_{\mathrm{z}x,y,z}$	

Heat flux

$R_n + \boldsymbol{L}E + H + G = 0$	for each canopy, snow, residue and soil surface, depending on exposure	[D11]
$G_{x(x,y,z)} = 2\ \kappa_{(x,y,z),(x+1,y,z)}\ (T_{(x,y,z)} - T_{(x+1,y,z)})/(\ L_{x\ (x,y,z)} + L_{x\ (x+1,y,z)}) + c_w\ T_{(x,y,z)}\ Q_{\mathrm{w}x(x,y,z)}$ $G_{y(x,y,z)} = 2\ \kappa_{(x,y,z),(x,y+1,z)}\ (T_{(x,y,z)} - T_{(x,y+1,z)})/(\ L_{y\ (x,y,z)} + L_{y\ (x,y+1,z)}) + c_w\ T_{(x,y,z)}\ Q_{\mathrm{w}y(x,y,z)}$ $G_{z(x,y,z)} = 2\ \kappa_{(x,y,z),(x,y,z+1)}\ (T_{(x,y,z)} - T_{(x,y,z+1)})/(\ L_{z\ (x,y,z)} + L_{z\ (x,y,z+1)}) + c_w\ T_{(x,y,z)}\ Q_{\mathrm{w}z(x,y,z)}$	3D conductive – convective heat flux among snowpack, surface residue and soil layers in *x* (EW), *y* (NS) and *z* (vertical) directions	[D12]

$G_{x(x-1,y,z)} - G_{x(x,y,z)} + G_{y(x,y-1,z)} - G_{y(x,y,z)} + G_{z(x,y,z-1)} - G_{z(x,y,z)} + \boldsymbol{L}Q_{f(x,y,z)} + c_{(x,y,z)} (T_{(x,y,z)} - T'_{(x,y,z)})/\Delta t = 0$	3D general heat flux equation in snowpack, surface residue and soil layers	[D13]

Gas flux

$Q_{\mathrm{ds}\gamma x,y,z} = a_{\mathrm{gs}x,y,z}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}\, [\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{ss}}]_{x,y,z})$	volatilization – dissolution between aqueous and gaseous phases in soil and root	[D14a]
$Q_{\mathrm{dr}\gamma x,y,z} = a_{\mathrm{gr}x,y,z}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}\, [\gamma_{\mathrm{gr}}]_{x,y,z} - [\gamma_{\mathrm{sr}}]_{x,y,z})$		[D14b]
$Q_{\mathrm{gs}\gamma\mathrm{z}x,y,1} = g_{\mathrm{a}x,y}\, \{[\gamma_{\mathrm{a}}] - \{2[\gamma_{\mathrm{gs}}]_{x,y,1} D_{\mathrm{gs}\gamma\mathrm{z}(x,y,1)}/L_{\mathrm{z}(x,y,1)} + g_{\mathrm{a}x,y}\, [\gamma_{\mathrm{a}}]]\}/\{2\, D_{\mathrm{gs}\gamma\mathrm{z}(x,y,1)}/L_{\mathrm{z}(x,y,1)} + g_{\mathrm{a}x,y}\}\}$	volatilization – dissolution between gaseous and aqueous phases at the soil surface ($z = 1$) and the atmosphere	[D15a]
$Q_{\mathrm{ds}\gamma x,y,1} = a_{\mathrm{gs}x,y,1}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,1}\, [\gamma_{\mathrm{a}}] - [\gamma_{\mathrm{ss}}]_{x,y,1})$		[D15b]

$$Q_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)} = - Q_{\mathrm{wx}(x,y,z)}\,[\gamma_{\mathrm{gs}}]_{x,y,z} + 2\,D_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)}\,([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x+1,y,z})/\,(L_{x\,(x,y,z)} + L_{x\,(x+1,y,z)}) \tag{D16a}$$

$$Q_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)} = - Q_{\mathrm{wy}(x,y,z)}\,[\gamma_{\mathrm{gs}}]_{x,y,z} + 2\,D_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)}\,([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x,y+1,z})/\,(L_{y\,(x,y,z)} + L_{y\,(x,y+1,z)}) \tag{D16b}$$

$$Q_{\mathrm{gs}\gamma\mathrm{z}(x,y,z)} = - Q_{\mathrm{wz}(x,y,z)}\,[\gamma_{\mathrm{gs}}]_{x,y,z} + 2\,D_{\mathrm{g}\gamma\mathrm{z}(x,y,z)}\,([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x,y,z+1})/\,(L_{z\,(x,y,z)} + L_{z\,(x,y,z+1)}) \tag{D16c}$$

3D convective - conductive gas flux among soil layers in *x* (EW), *y* (NS) and *z* (vertical) directions,

$$Q_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)} = D_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)}\,([\gamma_{\mathrm{gr}}]_{x,y,z} - [\gamma_{\mathrm{a}}])/\,\Sigma_{1,\mathrm{z}}\,L_{z\,(x,y,z)} \tag{D16d}$$

convective - conductive gas flux between roots and the atmosphere

$$D_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)} = \boldsymbol{D'}_{\mathbf{g}\gamma}\ f\mathrm{t}_{\mathrm{g}x,y,z}\,[0.5(\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x+1,y,z})]^2/\theta_{\mathrm{ps}x,y,z}{}^{0.67} \tag{D17a}$$

$$D_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)} = \boldsymbol{D'}_{\mathbf{g}\gamma}\ f\mathrm{t}_{\mathrm{g}x,y,z}\,[0.5(\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x,y+1,z})]^2/\theta_{\mathrm{ps}x,y,z}{}^{0.67} \tag{D17b}$$

$$D_{\mathrm{gs}\gamma\mathrm{z}(x,y,z)} = \boldsymbol{D'}_{\mathbf{g}\gamma}\ f\mathrm{t}_{\mathrm{g}x,y,z}\,[0.5(\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x,y,z+1})]^2/\theta_{\mathrm{ps}x,y,z}{}^{0.67} \tag{D17c}$$

gasous diffusivity as a function of air-filled porosity in soil

$$D_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)} = \boldsymbol{D'}_{\mathbf{g}\gamma}\ f\mathrm{t}_{\mathrm{g}x,y,z}\ \boldsymbol{\theta}_{\mathbf{pr}x,y,z}{}^{1.33}\,\mathrm{A}_{\mathrm{r}\,(x,y,z)}\,/\mathrm{A}_{x,y} \tag{D17d}$$

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

$$Q_{\mathrm{b}\gamma\mathrm{z}} = \min[0.0,\{(44.64\ \theta_{wx,y,z}\,273.16/T_{(x,y,z)}) - \Sigma_{\gamma}\,([\gamma_{\mathrm{s}}]_{x,y,z}/(\boldsymbol{S}'_{\gamma}\,f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}M_{\gamma}))\}] \\ ([\gamma_{\mathrm{s}}]_{x,y,z}/(\boldsymbol{S}'_{\gamma}\,f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}M_{\gamma}))/\,\Sigma_{\gamma}\,([\gamma_{\mathrm{s}}]_{x,y,z}/(\boldsymbol{S}'_{\gamma}\,f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}M_{\gamma}))\ \boldsymbol{S}'_{\gamma}\,f\mathrm{t}_{\mathrm{d}_{\gamma}x,y,z}M_{\gamma}\,V_{x,y,z} \tag{D18}$$

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

Solute flux

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

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

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

3D convective - dispersive solute flux among soil layers in *x* (EW), *y* (NS) and *z* (vertical) directions [D19]

$$D_{\mathrm{s}\gamma\mathrm{x}(x,y,z)} = D_{\mathrm{qx}(x,y,z)} \left| Q_{\mathrm{wx}(x,y,z)} \right| + \boldsymbol{D'}_{\mathrm{s}\gamma}\ ft_{\mathrm{s}x,y,z} [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$$

$$D_{\mathrm{s}\gamma\mathrm{y}(x,y,z)} = D_{\mathrm{qy}(x,y,z)} \left| Q_{\mathrm{wy}(x,y,z)} \right| + \boldsymbol{D'}_{\mathrm{s}\gamma}\ ft_{\mathrm{s}x,y,z} [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$$

$$D_{\mathrm{s}\gamma\mathrm{z}(x,y,z)} = D_{\mathrm{qz}(x,y,z)} \left| Q_{\mathrm{wz}(x,y,z)} \right| + \boldsymbol{D'}_{\mathrm{s}\gamma}\ ft_{\mathrm{s}x,y,z} [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$$

aqueous dispersivity as functions of water flux and water-filled porosity [D20]

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

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

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

dispersivity as a function of water flow length [D21]

Definition of variables in appendix D

Variable	Definition	Unit	Equation	Value	Reference
Subscripts					
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	
Variables					
A	area of landscape position	$\mathrm{m^2}$	[D17c]		
A_r	root cross-sectional area of landscape position	$\mathrm{m^2}$	[D17c]		
a_gr	air-water interfacial area in roots	$\mathrm{m^2\ m^{-2}}$	[D14b]		
a_gs	air-water interfacial area in soil	$\mathrm{m^2\ m^{-2}}$	[D14a,D15b]		Skopp (1985)
$\boldsymbol{\alpha}$	dependence of D_q on L	-	[D21]		
$\boldsymbol{\beta}$	dependence of D_q on L	-	[D21]		
c	heat capacity of soil	$\mathrm{MJ\ m^{-2}\ {}^{o}C^{-1}}$	[D13]		
c_w	heat capacity of water	$\mathrm{MJ\ m^{-3}\ {}^{o}C^{-1}}$	[D12]	4.19	
$D_{\mathrm{d}\gamma}$	volatilization - dissolution transfer coefficient for gas γ	$\mathrm{m^2\ h^{-1}}$	[D14,D15a]		

$D_{\mathrm{gr}\gamma}$	gaseous diffusivity of gas γ in roots	$\mathrm{m^2\ h^{-1}}$	[D16d,D17d]		Luxmoore et al. (1970a, b)
$D_{\mathrm{gs}\gamma}$	gaseous diffusivity of gas γ in soil	$\mathrm{m^2\ h^{-1}}$	[D15a,D16a,b,c,D17a,b,c]		Millington and Quirk (1960)
$\boldsymbol{D'}_{\mathrm{g}\gamma}$	diffusivity of gas γ in air at 0 $^{\mathrm{o}}$C	$\mathrm{m^2\ h^{-1}}$	[D17]	6.43 x 10^{-2} for $\gamma = \mathrm{O_2}$	Campbell (1985)
D_{q}	dispersivity	m	[D20,D21]		
$D_{\mathrm{s}\gamma}$	aqueous diffusivity of gas or solute γ	$\mathrm{m^2\ h^{-1}}$	[D19,D20]		
$\boldsymbol{D'}_{\mathrm{s}\gamma}$	diffusivity of gas γ in water at 0 $^{\mathrm{o}}$C	$\mathrm{m^2\ h^{-1}}$	[D20]	8.57 x 10^{-6} for $\gamma = \mathrm{O_2}$	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]		
WTD_x	external water table depth	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	$\mathrm{m^3\ m^{-2}\ h^{-1}}$	[D4,D11]		
e_{a}	atmospheric vapor density	$\mathrm{m^3\ m^{-3}}$	[D6]		

$e_{\mathrm{l}(T_l,\psi_l)}$	surface litter vapor density at current T_l and ψ_l	g m^{-3}	[D6a]	
$e_{\mathrm{s}(T_s,\psi_s)}$	soil surface vapor density at current T_s and ψ_s	g m^{-3}	[D6b]	
ft_{d_γ}	temperature dependence of $\boldsymbol{S}'_\gamma$	-	[D14,D15b,D18]	Wilhelm et al. (1977)
ft_g	temperature dependence of $\boldsymbol{D}'_{\mathbf{g}\gamma}$	-	[D17]	Campbell (1985)
ft_s	temperature dependence of $\boldsymbol{D}'_{\mathbf{s}\gamma}$	-	[D20]	Campbell (1985)
G	soil surface heat flux	m^3 m^{-2} h^{-1}	[D11]	
G_x, G_y, G_z	soil heat flux in x, y or z directions	MJ m^{-2} h^{-1}	[D12,D13]	
g_a	boundary layer conductance	m h^{-1}	[D15a]	
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]	
$[\gamma_\mathrm{a}]$	atmospheric concentration of gas γ	g m^{-3}	[D15,D16d]	
$[\gamma_\mathrm{gr}]$	gasous concentration of gas γ in roots	g m^{-3}	[D14b,D16d]	
$[\gamma_\mathrm{gs}]$	gasous concentration of gas γ in soil	g m^{-3}	[D14a,D15a,D16a ,D16b,D16c]	
$[\gamma_\mathrm{sr}]$	aqueous concentration of gas γ in roots	g m^{-3}	[D14b]	
$[\gamma_\mathrm{ss}]$	aqueous concentration of gas γ in soil	g m^{-3}	[D14a,D15b,D18, D19]	

H	sensible heat flux	MJ m^{-2} h^{-1}	[D11]		
K	hydraulic conductivity	m^2 MPa^{-1} h^{-1}	[D9]		Green and Corey (1971)
$Kmat$	soil matrix hydraulic conductivity	m^2 MPa^{-1} h^{-1}	[D10]		
$Kmac$	macropore hydraulic conductivity	m^2 MPa^{-1} h^{-1}	[D10a]		
K'_x , K'_y , K'_z	hydraulic conductance in x, y or z directions	m MPa^{-1} h^{-1}	[D7,D9]		
κ	thermal conductivity	MJ m^{-1} h^{-1} $^{o}C^{-1}$	[D12]		de Vries (1963)
L_t	distance from boundary to external water table in x or y directions	m	[D10]		
L_x , L_y , L_z	length of landscape element in x, y or z directions	m	[D1,D5b,D8,D9,D10,D12,D15a,D16,D19]		
$\boldsymbol{L}E_\mathrm{l}$	latent heat flux from surface litter	[D6a]	MJ m^{-2} h^{-1}		
$\boldsymbol{L}E_\mathrm{s}$	latent heat flux from soil surface	[D6b]	MJ m^{-2} h^{-1}		
$\boldsymbol{L}$	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	$m^3\ m^{-2}\ h^{-1}$	[D4]
$Q_{b\gamma z}$	bubbling flux	$g\ m^{-2}\ h^{-1}$	[D18]
$Q_{dr\gamma}$	volatilization – dissolution of gas γ between aqueous and gaseous phases in roots	$g\ m^{-2}\ h^{-1}$	[D14b]
$Q_{ds\gamma}$	volatilization – dissolution of gas γ between aqueous and gaseous phases in soil	$g\ m^{-2}\ h^{-1}$	[D14a,D15b]
Q_f	freeze-thaw flux (thaw +ve)	$m^3\ m^{-2}\ h^{-1}$	[D8,D13]
$Q_{gr\gamma}$	gaseous flux of gas γ between roots and the atmosphere	$g\ m^{-2}\ h^{-1}$	[D16d]
$Q_{gs\gamma}$	gaseous flux of gas γ in soil	$g\ m^{-2}\ h^{-1}$	[D15a,D16a,b,c]
Q_{rx}, Q_{ry}	surface water flow in x or y directions	$m^3\ m^{-2}\ h^{-1}$	[D1,D4]
$Q_{s\gamma}$	aqueous flux of gas or solute γ	$g\ m^{-2}\ h^{-1}$	[D19]
$Qmat_t$	water flux between boundary grid cell and external water table through soil matrix in x or y directions	$m^3\ m^{-2}\ h^{-1}$	[D10]
$Qmac_t$	water flux between boundary grid cell and external water table through macropores in x or y directions	$m^3\ m^{-2}\ h^{-1}$	[D10a]

$Q_{\mathrm{w}x},Q_{\mathrm{w}y},Q_{\mathrm{w}z}$	subsurface water flow in x, y or z directions	$\mathrm{m}^{3}\ \mathrm{m}^{-2}\ \mathrm{h}^{-1}$	[D4,D7,D8,D12,D16,D19,D20]		
θ_{g}	air-filled porosity	$\mathrm{m}^{3}\ \mathrm{m}^{-3}$	[D17a,b,c]		
θ_{mac}	macropore water content	$\mathrm{m}^{3}\ \mathrm{m}^{-3}$	[D10a]		
$\boldsymbol{\theta}_{\mathbf{pr}}$	root porosity	$\mathrm{m}^{3}\ \mathrm{m}^{-3}$	[D17d]	dryland spp. 0.10 wetland spp. 0.20	Luxmoore et al. (1970a, b)
θ_{ps}	soil porosity	$\mathrm{m}^{3}\ \mathrm{m}^{-3}$	[D17a,b,c]		
θ_{w}	water-filled porosity	$\mathrm{m}^{3}\ \mathrm{m}^{-3}$	[D8,D18,D20]		
R	ratio of cross-sectional area to perimeter of surface flow	m	[D3,D5a]		
R_{n}	net radiation	$\mathrm{MJ\ m}^{-2}\ \mathrm{h}^{-1}$	[D11]		
$r_{\mathrm{a}l}$	surface litter boundary layer resistance	$\mathrm{m\ h}^{-1}$	[D6a]		
$r_{\mathrm{a}s}$	Soil surface boundary layer resistance	$\mathrm{m\ h}^{-1}$	[D6b]		
$\boldsymbol{S}'_{\gamma}$	Ostwald solubility coefficient of gas γ at 30 $^{\mathrm{o}}$C	-	[D14,D15b,D18]	0.0293 for $\gamma = \mathrm{O}_2$	Wilhelm et al. (1977)
s_{r}	slope of channel sides during surface flow	$\mathrm{m\ m}^{-1}$	[D5a]		
s_{x} , s_{y}	slope in x or y directions	$\mathrm{m\ m}^{-1}$	[D3,D5b]		

T	soil temperature	^{o}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]	-2.0 x 10^{-2}
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

$Al(OH)_{3(s)} \Leftrightarrow (Al^{3+}) + 3\ (OH^{-})$	(amorphous $Al(OH)_3$)	*-33.0*	[E.1] [1]
$Fe(OH)_{3(s)} \Leftrightarrow (Fe^{3+}) + 3\ (OH^{-})$	(soil Fe)	*-39.3*	[E.2]
$CaCO_{3(s)} \Leftrightarrow (Ca^{2+}) + (CO_3^{2-})$	(calcite)	-9.28	[E.3]
$CaSO_{4(s)} \Leftrightarrow (Ca^{2+}) + (SO_4^{2-})$	(gypsum)	*-4.64*	[E.4]
$AlPO_{4(s)} \Leftrightarrow (Al^{3+}) + (PO_4^{3-})$	(variscite)	*-22.1*	[E.5] [2]

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[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 equlilibrium 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.

$FePO_{4(s)} \Leftrightarrow (Fe^{3+}) + (PO_4^{3-})$ (strengite) *-26.4* [E.6]

$Ca(H_2PO_4)_{2(s)} \Leftrightarrow (Ca^{2+}) + 2\,(H_2PO_4^{-})$ (monocalcium phosphate) *-1.15* [E.7][3]

$CaHPO_{4(s)} \Leftrightarrow (Ca^{2+}) + (HPO_4^{2-})$ (monetite) *-6.92* [E.8]

$Ca_5(PO_4)_3OH_{(s)} \Leftrightarrow 5\,(Ca^{2+}) + 3\,(PO_4^{3-}) + (OH^{-})$ (hydroxyapatite) *-58.2* [E.9]

Cation exchange equilibria [4]

$X\text{-}Ca + 2\,(NH_4^{+}) \Leftrightarrow 2\,X\text{-}NH_4 + (Ca^{2+})$ *1.00* [E.10]

$3\,X\text{-}Ca + 2\,(Al^{3+}) \Leftrightarrow 2\,X\text{-}Al + 3\,(Ca^{2+})$ *1.00* [E.11]

$X\text{-}Ca + (Mg^{2+}) \Leftrightarrow X\text{-}Mg + (Ca^{2+})$ *0.60* [E.12]

$X\text{-}Ca + 2\,(Na^{+}) \Leftrightarrow 2\,X\text{-}Na + (Ca^{2+})$ *0.16* [E.13]

$X\text{-}Ca + 2\,(K^{+}) \Leftrightarrow 2\,X\text{-}K + (Ca^{2+})$ *3.00* [E.14]

$X\text{-}Ca + 2\,(H^{+}) \Leftrightarrow 2\,X\text{-}H + (Ca^{2+})$ *1.00* [E.15]

Anion adsorption equilibria

$X\text{-}OH_2^{+} \Leftrightarrow X\text{-}OH + (H^{+})$ *-7.35* [E.16]

$X\text{-}OH \Leftrightarrow X\text{-}O^{-} + (H^{+})$ *-8.95* [E.17]

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[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.

$X\text{-}H_2PO_4 + H_2O \Leftrightarrow X\text{-}OH_2^{+} + (H_2PO_4^{-})$ *-2.80* [E.18]

$X\text{-}H_2PO_4 + (OH^{-}) \Leftrightarrow X\text{-}OH + (H_2PO_4^{-})$ *4.20* [E.19]

$X\text{-}HPO_4^{-} + (OH^{-}) \Leftrightarrow X\text{-}OH + (HPO_4^{2-})$ *2.60* [E.20]

Organic acid equilibria

$X\text{-}COOH \Leftrightarrow X\text{–}COO^{-} + (H^{+})$ *-5.00* [E.21]

Ion pair equilibria

$(NH_4^{+}) \Leftrightarrow (NH_3)_{(g)} + (H^{+})$ *-9.24* [E.22]

$H_2O \Leftrightarrow (H^{+}) + (OH^{-})$ *-14.3* [E.23]

$(CO_2)_{(g)} + H_2O \Leftrightarrow (H^{+}) + (HCO_3^{-})$ *-6.42* [E.24]

$(HCO_3^{-}) \Leftrightarrow (H^{+}) + (CO_3^{2-})$ *-10.4* [E.25]

$(AlOH^{2+}) \Leftrightarrow (Al^{3+}) + (OH^{-})$ *-9.06* [E.26]

$(Al(OH)_2^{+}) \Leftrightarrow (AlOH^{2+}) + (OH^{-})$ *-10.7* [E.27]

$(Al(OH)_3^{0}) \Leftrightarrow (Al(OH)_2^{+}) + (OH^{-})$ *-5.70* [E.28]

$(Al(OH)_4^{-}) \Leftrightarrow (Al(OH)_3^{0}) + (OH^{-})$ *-5.10* [E.29]

$(AlSO_4^{+}) \Leftrightarrow (Al^{3+}) + (SO_4^{2-})$ *-3.80* [E.30]

$(FeOH^{2+}) \Leftrightarrow (Fe^{3+}) + (OH^{-})$ *-12.1* [E.31]

$(Fe(OH)_2^{+}) \Leftrightarrow (FeOH^{2+}) + (OH^{-})$ *-10.8* [E.32]

$(Fe(OH)_3^{0}) \Leftrightarrow (Fe(OH)_2^{+}) + (OH^{-})$ *-6.94* [E.33]

$(Fe(OH)_4^{-}) \Leftrightarrow (Fe(OH)_3^{0}) + (OH^{-})$ *-5.84* [E.34]

$(FeSO_4^{+}) \Leftrightarrow (Fe^{3+}) + (SO_4^{2-})$ *-4.15* [E.35]

$(CaOH^{+}) \Leftrightarrow (Ca^{2+}) + (OH^{-})$ *-1.90* [E.36]

$(CaCO_3^{0}) \Leftrightarrow (Ca^{2+}) + (CO_3^{2-})$ *-4.38* [E.37]

$(CaHCO_3^{+}) \Leftrightarrow (Ca^{2+}) + (HCO_3^{-})$ *-1.87* [E.38]

$(CaSO_4^{0}) \Leftrightarrow (Ca^{2+}) + (SO_4^{2-})$ *-2.92* [E.39]

$(MgOH^{+}) \Leftrightarrow (Mg^{2+}) + (OH^{-})$ *-3.15* [E.40]

$(MgCO_3^{0}) \Leftrightarrow (Mg^{2+}) + (CO_3^{2-})$ *-3.52* [E.41]

$(MgHCO_3^{+}) \Leftrightarrow (Mg^{2+}) + (HCO_3^{-})$ *-1.17* [E.42]

$(MgSO_4^{0}) \Leftrightarrow (Mg^{2+}) + (SO_4^{2-})$ *-2.68* [E.43]

$(NaCO_3^{-}) \Leftrightarrow (Na^{+}) + (CO_3^{2-})$ *-3.35* [E.44]

$(NaSO_4^{-}) \Leftrightarrow (Na^{+}) + (SO_4^{2-})$ *-0.48* [E.45]

$(KSO_4^{-}) \Leftrightarrow (K^{+}) + (SO_4^{2-})$ *-1.30* [E.46]

$(H_3PO_4) \Leftrightarrow (H^{+}) + (H_2PO_4^{-})$ *-2.15* [E.47]

$(H_2PO_4^{-}) \Leftrightarrow (H^{+}) + (HPO_4^{2-})$ *-7.20* [E.48]

$(HPO_4^{2-}) \Leftrightarrow (H^{+}) + (PO_4^{3-})$ *-12.4* [E.49]

$(FeH_2PO_4^{2+}) \Leftrightarrow (Fe^{3+}) + (H_2PO_4^{-})$ *-5.43* [E.50]

$(FeHPO_4^{+}) \Leftrightarrow (Fe^{3+}) + (HPO_4^{2-})$ *-10.9* [E.51]

$(CaH_2PO_4^{+}) \Leftrightarrow (Ca^{2+}) + (H_2PO_4^{-})$ *-1.40* [E.52]

$(CaHPO_4^{0}) \Leftrightarrow (Ca^{2+}) + (HPO_4^{2-})$ *-2.74* [E.53]

$(CaPO_4^{-}) \Leftrightarrow (Ca^{2+}) + (PO_4^{3-})$ *-6.46* [E.54]

$(MgHPO_4^{0}) \Leftrightarrow (Mg^{2+}) + (HPO_4^{2-})$ *-2.91* [E.55]

Appendix F: Symbiotic N$_2$ fixation

Rhizobial growth

$R_{\mathrm{max}i,l} = M_{\mathrm{n}i,l}\, R'\, [\chi_{\mathrm{n}i,l}]/([\chi_{\mathrm{n}i,l}] + K_{\chi\mathrm{n}})\, f_{\mathrm{t}}\, f_{\mathrm{NP}}$ respiration demand [F1]

$f_{\mathrm{t}} = T_l\{\exp[B - H_{\mathrm{a}}/(RT_l)]\}/\{1 + \exp[(H_{\mathrm{dl}} - ST_l)/(RT_l)] + \exp[(ST_l - H_{\mathrm{dh}})/(RT_l)]\}$ Arrhenius function [F2]

$f_{\mathrm{NP}} = \min\{[N_{\mathrm{n}i,l}]/[N_{\mathrm{n}}'], [P_{\mathrm{n}i,l}]/[P_{\mathrm{n}}']\}$ N or P limitation [F3]

$R_{i,l} = R_{\mathrm{max}i,l}\ (V_{\mathrm{O_2}i,l}/V_{\mathrm{O_2max}i,l})$	O_2 limitation		[F4]
$V_{\mathrm{O_2max}i,l} = 2.67\ R_{\mathrm{max}i,l}$	O_2 demand		[F5]
$V_{\mathrm{O_2}i,l} = V_{\mathrm{O_2max}i,l}\ [\mathrm{O}_{2\mathrm{r}i,l}]/([\mathrm{O}_{2\mathrm{r}i,l}] + K_{\mathrm{O_2r}})$	equilibrate O_2 uptake with supply		[F6a]
$= 2\pi L_{\mathrm{r}i,l}\ D_{\mathrm{sO_2}}\ ([\mathrm{O}_{2l}] - [\mathrm{O}_{2\mathrm{r}i,l}])/\ln((r_{\mathrm{r}i,l} + \mathrm{r}_{\mathrm{w}l}))/\mathrm{r}_{\mathrm{r}i,l})$			[F6b]
$R_{\mathrm{m}i,l} = \boldsymbol{R}_\mathrm{m}\ N_{\mathrm{n}i,l} f_\mathrm{tm}$	maintenance respiration		[F7]
$f_\mathrm{tm} = e^{[y(T_l - 298.16)]}$	temperature function		[F8]
$R_{\mathrm{g}i,l} = \max\{0.0, R_{i,l} - R_{\mathrm{m}i,l}\}$	growth + fixation respiration		[F9]
$R_{\mathrm{s}i,l} = \max\{0.0, R_{\mathrm{m}i,l} - R_{i,l}\}$	microbial senescence		[F10]
$L_{Ci,l} = R_{\mathrm{s}i,l}\ \min\{M_{\mathrm{n}i,l}/(2.5N_{\mathrm{n}i,l}), M_{\mathrm{n}i,l}/(25.0P_{\mathrm{n}i,l})\}$	microbial C litterfall		[F11]

N_2 fixation

$V_{\mathrm{N_2}i,l} = \min\{R_{\mathrm{g}i,l}\ E_{\mathrm{N_2}}'\ f_\mathrm{CP}, M_{\mathrm{n}i,l}\ [N_\mathrm{n}'] - N_{\mathrm{n}i,l}\}\ [\mathrm{N}_{2\mathrm{r}i,l}]/([\mathrm{N}_{2\mathrm{r}i,l}] + K_{\mathrm{N_2r}})$	rate of N_2 fixation		[F12]
$f_\mathrm{CP} = \min\{[\chi_{\mathrm{n}i,l}]/(1.0 + [\nu_{\mathrm{n}i,l}]/K_{\mathrm{I}\chi_\mathrm{n}}), [\pi_{\mathrm{n}i,l}]/(1.0 + [\nu_{\mathrm{n}i,l}]/K_{\mathrm{I}\pi_\mathrm{n}})\}$	product inhibition of N_2 fixation		[F13]
$R_{\mathrm{N_2}i,l} = V_{\mathrm{N_2}i,l}/E_{\mathrm{N_2}}'$	fixation respiration		[F14]
$U_{\chi i,l} = (R_{\mathrm{g}i,l} - R_{\mathrm{N_2}i,l})/(1 - Y_\mathrm{n}')$	growth respiration		[F15]
$\delta M_{\mathrm{n}i,l}/\delta t = U_{i,l}\ Y_\mathrm{n}' - L_{Ci,l}$	microbial C growth		[F16]
$\delta N_{\mathrm{n}i,l}/\delta t = \delta M_{\mathrm{n}i,l}/\delta t\ \min\{\nu_{\mathrm{n}i,l}/\chi_{\mathrm{n}i,l}, [N_\mathrm{n}']\}$	microbial N growth	$\delta M_{\mathrm{nd}i,l}/\delta t > 0$	[F17a]

$\delta N_{\mathrm{n}i,l}/\delta t = N_{\mathrm{n}i,l}/M_{\mathrm{n}i,l}\ \delta M_{\mathrm{n}i,l}/\delta t$	microbial N growth	$\delta M_{\mathrm{nd}i,l}/\delta t < 0$	[F17b]
$\delta P_{\mathrm{n}i,l}/\delta t = \delta M_{\mathrm{n}i,l}/\delta t\ \min\{\pi_{\mathrm{n}i,l}/\chi_{\mathrm{n}i,l}, [P_{\mathrm{n}}']\}$	microbial P growth	$\delta M_{\mathrm{nd}i,l}/\delta t > 0$	[F18a]
$\delta P_{\mathrm{n}i,l}/\delta t = P_{\mathrm{n}i,l}/M_{\mathrm{n}i,l}\ \delta M_{\mathrm{n}i,l}/\delta t$	microbial P growth	$\delta M_{\mathrm{nd}i,l}/\delta t < 0$	[F18b]
$L_{Ni,l} = \mathrm{abs}(\delta N_{\mathrm{n}i,l}/\delta t)$	microbial N litterfall	$\delta N_{\mathrm{nd}i,l}/\delta t < 0$	[F19]
$L_{Pi,l} = \mathrm{abs}(\delta P_{\mathrm{n}i,l}/\delta t)$	microbial P litterfall	$\delta P_{\mathrm{nd}i,l}/\delta t < 0$	[F20]

Nodule-root exchange

$V_{\chi i,l} = \kappa\,(\chi_{\mathrm{r}i,l}\,M_{\mathrm{n}i,l} - \chi_{\mathrm{n}i,l}\,M_{\mathrm{r}i,l})/(M_{\mathrm{n}i,l} + M_{\mathrm{r}i,l})$	nodule–root C exchange		[F21]
$V_{\nu i,l} = \kappa\,(\nu_{\mathrm{r}i,l}\,\chi_{\mathrm{n}i,l} - \nu_{\mathrm{n}i,l}\,\chi_{\mathrm{r}i,l})/(\chi_{\mathrm{n}i,l} + \chi_{\mathrm{r}i,l})$	nodule–root N exchange		[F22]
$V_{\pi i,l} = \kappa\,(\pi_{\mathrm{r}i,l}\,\chi_{\mathrm{n}i,l} - \pi_{\mathrm{n}i,l}\,\chi_{\mathrm{r}i,l})/(\chi_{\mathrm{n}i,l} + \chi_{\mathrm{r}i,l})$	nodule–root P exchange		[F23]
$\delta \chi_{\mathrm{n}i,l}/\delta t = V_{\chi i,l} - \min\{R_{\mathrm{m}i,l}, R_{i,l}\} - R_{\mathrm{N}_2 i,l} - U_{\chi i,l} + F_{LC\,l}\,L_{Ci,l}$	nodule nonstructural C		[F24]
$\delta \nu_{\mathrm{n}i,l}/\delta t = V_{\nu i,l} - \delta N_{\mathrm{n}i,l}/\delta t + V_{\mathrm{N}_2 i,l} + F_{LN\,l}\,L_{Ni,l}$	nodule nonstructural N		[F25]
$\delta \pi_{\mathrm{n}i,l}/\delta t = V_{\pi i,l} - \delta P_{\mathrm{n}i,l}/\delta t + F_{LP\,l}\,L_{Pi,l}$	nodule nonstructural P		[F26]

Definition of variables in appendix F

Variable	Definition	Units	Equations	Input Values	Reference
B	parameter such that $f_{\mathrm{t}} = 1.0$ at $T_l = 298.15$ K		F2	17.533	

$\chi_{\mathrm{n}i,l}$	nodule nonstructural C	g m^{-2}	F17a,F18a,F21,F22,B23,B24		
$[\chi_{\mathrm{n}i,l}]$	nodule nonstructural C concentration	g g^{-1}	F1,F13		
$\chi_{\mathrm{r}i,l}$	root nonstructural C	g m^{-2}	F21,F22,F23		
D_{sO_2}	diffusivity of aqueous O_2	m^2 h^{-1}	F6b		
E_{N_2}'	direct energy cost of N_2 fixation	g N g C^{-1}	F12,F14	0.25	Gutschick (1981), Voisin et al. (2003)
$F_{LC\ l}$	fraction of nodule C litterfall remobilized as nonstructural C	-	F24		
$F_{LN\ l}$	fraction of nodule N litterfall remobilized as nonstructural N	-	F25		
$F_{LP\ l}$	fraction of nodule P litterfall remobilized as nonstructural P	-	F26		
f_{CP}	effect of nodule nonstructural C or P content on N_2 fixation	-	F12,F13		
f_{NP}	effect of nodule N or P content on respiration	-	F1,F3		
f_{t}	temperature function for nodule respiration	-	F1,F2		
f_{tm}	temperature function for nodule maintenance respiration	-	F7,F8		

H_{a}	energy of activation	J mol^{-1}	F2	57.5 x 10^{3}
H_{dh}	energy of high temperature deactivation	J mol^{-1}	F2	220 x 10^{3}
H_{dl}	energy of low temperature deactivation	J mol^{-1}	F2	190 x 10^{3}
$K_{\chi\mathrm{n}}$	Michaelis-Menten constant for nodule respiration of $\chi_{\mathrm{nd}i,l}$	g g^{-1}	F1	0.01
$K_{\mathrm{I}\chi_{\mathrm{n}}}$	inhibition constant for nonstructural N:C on N_2 fixation	g g^{-1}	F13	10
$K_{\mathrm{I}\pi_{\mathrm{n}}}$	inhibition constant for nonstructural N:P on N_2 fixation	g g^{-1}	F13	1000
$K_{\mathrm{N_2r}}$	Michaelis-Menten constant for nodule N_2 uptake	g N m^{-3}	F12	0.14
$K_{\mathrm{O_2r}}$	Michaelis-Menten constant for nodule O_2 uptake	g O m^{-3}	F6a	
κ	rate constant for nonstructural C,N,P exchange between root and nodule	h^{-1}	F21,F22,F23	
$L_{\mathrm{r}i,l}$	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	

$M_{\mathrm{n}i,l}$	nodule structural C	g C m^{-2}	F1,F11,F12,F16,F17,F18,F21	
$M_{\mathrm{r}i,l}$	root structural C	g C m^{-2}	F21	
$[N_{\mathrm{n}}']$	maximum nodule structural N concentration	g N g C^{-1}	F3,F12	0.1
$N_{\mathrm{n}i,l}$	nodule structural N	g N m^{-2}	F7,F11,F12,F17,F19,F25	
$[N_{\mathrm{n}i,l}]$	nodule structural N concentration	g N g C^{-1}	F3,F17a	
$[\mathrm{N}_{2\mathrm{r}i,l}]$	rhizosphere aqueous N_2 concentration	g N m^{-3}	F12	
$\nu_{\mathrm{n}i,l}$	nodule nonstructural N	g N m^{-2}	F17a,F22,F25	
$\nu_{\mathrm{r}i,l}$	root nonstructural N	g N m^{-2}	F22	
$[\nu_{\mathrm{n}i,l}]$	nodule concentration of nonstructural N	g g^{-1}	F13,F17a	
$[\mathrm{O}_{2\mathrm{r}i,l}]$	rhizosphere aqueous O_2 concentration	g O m^{-3}	F6a,b	
$[\mathrm{O}_{2l}]$	soil aqueous O_2 concentration	g O m^{-3}	F6b	
$[P_{\mathrm{n}}']$	maximum nodule structural P concentration	g P g C^{-1}	F3,F18a	0.01

$P_{\mathrm{n}i,l}$	nodule structural P	$\mathrm{g\ P\ m^{-2}}$	F18a,F20,F26	
$[P_{\mathrm{n}i,l}]$	nodule structural P concentration	$\mathrm{g\ P\ g\ C^{-1}}$	F3,F11	
$\pi_{\mathrm{n}i,l}$	nodule nonstructural P	$\mathrm{g\ P\ m^{-2}}$	F18a,F23,F26	
$\pi_{\mathrm{r}i,l}$	root nonstructural P	$\mathrm{g\ P\ m^{-2}}$	F23	
$[\pi_{\mathrm{n}i,l}]$	nodule concentration of nonstructural P	$\mathrm{g\ g^{-1}}$	F13	
R	gas constant	$\mathrm{J\ mol^{-1}\ K^{-1}}$	F2	8.3143
$R_{\mathrm{g}i,l}$	nodule growth respiration	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	F9,F12,F15	
R'	specific nodule respiration at 25°C, and non-limiting O_2, $\chi_{\mathrm{nd}i,l}$, $\nu_{\mathrm{nd}i,l}$ and $\pi_{\mathrm{nd}i,l}$	$\mathrm{h^{-1}}$	F1	0.125
$R_{i,l}$	nodule respiration under ambient O_2	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	F4,F9,F10,F24	
$\boldsymbol{R}_{\mathrm{m}}$	specific nodule maintenance respiration at 25°C	$\mathrm{g\ C\ g\ C^{-1}\ h^{-1}}$	F7	
$R_{\mathrm{max}i,l}$	nodule respiration under non-limiting O_2	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	F1,F4,F5	
$R_{\mathrm{m}i,l}$	nodule maintenance respiration	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	F7,F9,F10,F24	
$R_{\mathrm{N_2}i,l}$	nodule respiration for N_2 fixation	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	F14,F15,F24	

$R_{\mathrm{s}i,l}$	nodule senescence respiration	g C m^{-2} h^{-1}	F9,F11	
$r_{\mathrm{r}i,l}$	root radius	m	F6b	
$\mathrm{r}_{\mathrm{w}l}$	radius of soil water films	m	F6b	
S	change in entropy	J mol^{-1} K^{-1}	F2	710
T_l	soil temperature	K	F2,F8	
$U_{\chi i,l}$	uptake of nodule nonstructural C for growth	g C m^{-2} h^{-1}	F15,F16,F24	
$V_{\chi i,l}$	nonstructural C transfer between root and nodule	g C m^{-2} h^{-1}	F21,F24	
$V_{\nu i,l}$	nonstructural N transfer between root and nodule	g N m^{-2} h^{-1}	F22,F25	
$V_{\mathrm{N_2}i,l}$	N_2 fixation	g N m^{-2} h^{-1}	F12,F14,F25	
$V_{\mathrm{O_2max}i,l}$	O_2 uptake by nodules under non-limiting O_2	g O m^{-2} h^{-1}	F4,F5,F6a	
$V_{\mathrm{O2}i,l}$	O_2 uptake by nodules under ambient O_2	g O m^{-2} h^{-1}	F4,F6	
$V_{\pi i,l}$	nonstructural P transfer between root and nodule	g P m^{-2} 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: CH_4 production and consumption

Anaerobic fermenters and H_2 producing acetogens

$\mathrm{R}i,f\ =\ \{\boldsymbol{R'f}\ \mathrm{M}i,f,a\ [\mathrm{DOC}i,c]/(\mathbf{K}\boldsymbol{f}\ ((1+[\mathrm{O}_2]/\mathbf{K}_i) + [\mathrm{DOC}i,c])\}\ \mathrm{ft}$	respiration by fermenters		[G1]
$\mathrm{DOC}i,c \rightarrow 0.67\ \mathrm{A}_{i,c} + 0.33\ \mathrm{CO_2\text{-}C} + 0.11\ \mathrm{H_2}$	partition respiration products		[G2]
$\mathrm{U}i,f,c\ = \mathrm{Rm}i,f + (\mathrm{R}i,f - \mathrm{Rm}i,f)(1.0 + \mathrm{Y}f)$	uptake by fermenters	$[\mathrm{R}i,f\ > \mathrm{Rm}i,f]$	[G3a]
$\mathrm{U}i,f,c\ = \mathrm{R}i,f$		$[\mathrm{R}i,f\ < \mathrm{Rm}i,f]$	[G3b]
$\mathrm{Y}f\ = -\Delta \mathrm{G}f\,/\,\mathbf{E_M}$	growth yield of fermentation		[G4]
$\Delta \mathrm{G}f\ = \boldsymbol{\Delta G'f}\ + \{\boldsymbol{R}\mathrm{Tln}([\mathrm{H_2}]/\mathbf{[H_2']})^4\}$	free energy change of fermentation		[G5]
$\delta \mathrm{M}i,f,j,c/\delta \mathrm{t} = \mathrm{F}j\ \mathrm{U}i,f,c - \mathrm{F}j\ \mathrm{R}i,f - \mathrm{D}i,f,j,c$	growth of fermenters	$[\mathrm{R}i,f\ > \mathrm{Rm}i,f]$	[G6a]
$\delta \mathrm{M}i,f,j,c/\delta \mathrm{t} = \mathrm{F}j\ \mathrm{U}i,f,c - \mathrm{Rm}i,f,j - \mathrm{D}i,f,j,c$		$[\mathrm{R}i,f\ < \mathrm{Rm}i,f]$	[G6b]

Acetotrophic methanogens

$\mathrm{R}_{i,m}\ =\ \{\boldsymbol{R'_m}\ \mathrm{M}_{i,m,a}\ [\mathrm{A}_{i,c}]/(\mathbf{K}_{\boldsymbol{m}} + [\mathrm{A}_{i,c}])\}\ \mathrm{f_t}$	respiration by acetotrophic methanogens		[G7]
$\mathrm{A}i,c \rightarrow\ 0.50\ \mathrm{CH_4\text{-}C} + 0.50\ \mathrm{CO_2\text{-}C}$	partition respiration products		[G8]
$\mathrm{U}_{i,m,c}\ = \mathrm{R}_{\mathrm{m}i,m} + (\mathrm{R}_{i,m} - \mathrm{R}_{\mathrm{m}i,m})(1.0 + \mathrm{Y}_m)$	uptake by acetotrophic methanogens	$[\mathrm{R}_{i,m} > \mathrm{R}_{\mathrm{m}i,m}]$	[G9a]

$U_{i,m,c} = R_{i,m}$		$[R_{i,m} < R_{\mathrm{m}i,m}]$	[G9b]
$-Y_m = -\boldsymbol{\Delta G'_m} / \mathbf{E_M}$	growth yield of acetotrophic methanogenesis		[G10]
$\delta M_{i,m,j,c}/\delta t = F_j U_{i,m,c} - F_j R_{i,m} - D_{i,m,j,c}$	growth of acetotrophic methanogens	$[R_{i,m} > R_{\mathrm{m}i,m}]$	[G11a]
$\delta M_{i,m,j,c}/\delta t = F_j U_{i,m,c} - R_{\mathrm{m}i,m,j} - D_{i,m,j,c}$		$[R_{i,m} < R_{\mathrm{m}i,m}]$	[G11b]

Hydrogenotrophic methanogens

$R_h = \{\boldsymbol{R'_h} M_{h,a} [H_2]/(\mathbf{K_h} + [H_2]) [CO_2]/(\mathbf{K_c} + [CO_2])\} f_t$	respiration by hydrogenotrophic methanogens		[G12]
$CO_2\text{-}C + 0.67\ H_2 \rightarrow CH_4\text{-}C + 3\ H_2O$	partition respiration products		[G13]
$U_{h,c} = R_{\mathrm{m}h} + (R_h - R_{\mathrm{m}h})(1.0 + Y_h)$	uptake by hydrogenotrophic methanogens	$[R_h > R_{\mathrm{m}h}]$	[G14a]
$U_{h,c} = R_h$		$[R_h < R_{\mathrm{m}h}]$	[G14b]
$Y_h = -\Delta G_h/\mathbf{E_C}$	growth yield of hydrogenotrophic methanogenesis		[G15]
$\Delta G_h = \boldsymbol{\Delta G'_h} - \{\boldsymbol{R}T\ln([H_2]/\mathbf{[H_2']})^4\}$	free energy change of hydrogenotrophic methanogenesis		[G16]

$\delta M_{h,j,c}/\delta t = F_j U_{h,c} - F_j R_h - D_{h,j,c}$	growth of hydrogenotrophic methanogens	$[R_h > R_{mh}]$	[G17a]
$\delta M_{h,j,c}/\delta t = F_j U_{h,c} - R_{mh,j} - D_{h,j,c}$		$[R_h < R_{mh}]$	[G17b]

Autotrophic methanotrophs

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

$CH_2O\text{-}C + 2.67\ O_2 \rightarrow CO_2\text{-}C + 1.5\ H_2O$ O_2 requirements for respiration by methanotrophs [G24]

$U_{t,c} = R_{mt} + (R_t - R_{mt})(1.0 + Y_{t_G})$ uptake by methanotrophs $[R_t > R_{mt}]$ [G25a]

$U_{t,c} = R_t$ $[R_t < R_{mt}]$ [G25b]

$Y_{t_G} = \mathbf{-\Delta G'_{\mathit{c}} / E_M}$ 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]		
a	descriptor for j = active component of Mi				
$[CH_4]$	aqueous concentration of CH_4	$g\ C\ m^{-3}$	[G18]		
$[CO_2]$	aqueous concentration of CO_2	$g\ C\ m^{-3}$	[G12]		
Dh,j,c	decomposition of hydrogenotrophic methanogens	$g\ C\ m^{-2}\ h^{-1}$	[G17]		

$\mathrm{D}i,f,j,c$	decomposition of fermenters and acetogens	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	[G6]		
$\mathrm{D}i,m,j,c$	decomposition of acetotrophic methanogens	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	[G11]		
$\mathrm{D}t,j,c$	decomposition of autotrophic methanotrophs	$\mathrm{g\ C\ m^{-2}\ h^{-1}}$	[G27]		
$\mathbf{E_C}$	energy required to construct new M from CO_2	$\mathrm{kJ\ g\ C^{-1}}$	[G15]	75	
$\mathbf{E_G}$	energy required to transform CH_4 into organic C	$\mathrm{kJ\ g\ C^{-1}}$	[G20]	23.5	Anthony (1982)
$\mathbf{E_M}$	energy required to construct new M from organic C	$\mathrm{kJ\ g\ C^{-1}}$	[G4,G10,G26]	25	
$\mathrm{F}j$	partitioning coefficient for j in $\mathrm{M}i,n,j$		[G6,G11,G17,G27]		
f	descriptor for fermenters and acetogens in each M_i				
fo_2t	ratio of O_2 uptake to O_2 requirement for CH_4 oxidation		[G21a,b]		
$\mathrm{f_t}$	temperature function for growth-related processes (dimensionless)		[G1,G7,G12]		
$\boldsymbol{\Delta G'_c}$	free energy change of C oxidation-O_2 reduction	$\mathrm{kJ\ g\ C^{-1}}$	[G26]	-37.5	Brock and Madigan (1991)

ΔG_f	free energy change of fermentation plus acetogenesis	kJ g $P_{i,c}^{-1}$	[G4,G5]		
$\Delta G'_f$	ΔG_f when $[H_2] = [H_2']$	kJ g $P_{i,c}^{-1}$	[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	Brock and Madigan (1991), Schink (1997)
$\Delta G'_t$	free energy change of CH_4 oxidation by methanotrophs	kJ g CH_4-C^{-1}	[G20]	-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]	150×10^{-6}	Brock and Madigan (1991)
h	descriptor for hydrogenotrophic methanogens in each M_i				
i	descriptor for organic matter-microbe complex (i = plant residue, manure, particulate OM, or humus)				
j	descriptor for structural or kinetic components for each functional type within each M_i *(e.g. a = active)*				
K_c	M-M constant for uptake of CO_2 by hydrogenotrophic methanogens	g C m^{-3}	[G12]	0.12	
K_f	M-M constant for uptake of $DOC_{i,c}$ by fermenters and acetogens	g C m^{-3}	[G1]	12	McGill et al. (1981)
K_i	inhibition constant for O_2 on fermentation	g O m^{-3}	[G1]	0.064	
K_h	M-M constant for uptake of H_2 by hydrogenotrophic methanogens	g H m^{-3}	[G12]	0.01	Robinson and Tiedje (1982), Mosey (1983)

$\mathbf{K}_{\boldsymbol{m}}$	M-M constant for uptake of $A_{i,c}$ by acetotrophic methanogens	g C m^{-3}	[G7]	12	Smith and Mah (1978), Zehnder et al. (1980)
$\mathbf{K}_{\boldsymbol{t}}$	M-M constant for uptake of CH_4 by methanotrophs	g C m^{-3}	[G18]	3×10^{-3}	Conrad (1984)
k	descriptor for elemental fraction within each j ($j = c, n$ or p)				
M	microbial communities	g C m^{-2}			
M_h	hydrogenotrophic methanogen community	g C m^{-2}	[G12,G17]		
$M_{i,f}$	fermenter and acetogenic community	g C m^{-2}	[G1,G6]		
$M_{i,m}$	acetotrophic methanogen community	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				
DOC	soluble organic matter	g C m^{-2}	[G2]		
[DOC]	aqueous concentration of soluble organic matter	g C m^{-3}	[G1]		
$\boldsymbol{R}$	gas constant	kJ mol^{-1} K^{-1}	[G5,G16]	8.3143×10^{-3}	

$\boldsymbol{R'_f}$	specific respiration by fermenters and acetogens at saturating [$P_{i,c}$], 30 °C and zero water potential	g C g $M_{i,f,a}^{-1}$ h^{-1}	[G1]	0.4	Lawrence (1971), Wofford et al. (1986)
R_h	CO_2 reduction by hydrogenotrophic methanogens	g C m^{-2} h^{-1}	[G12,G13,G14,G17,G18]		
$\boldsymbol{R'_h}$	specific CO_2 reduction by hydrogenotrophic methanogens at saturating [H_2] and [CO_2], and at 30 °C and zero water potential	g C g $M_{h,a}^{-1}$ h^{-1}	[G12]	0.12	Shea et al. (1968), Zehnder and Wuhrmann (1977)
$R_{i,f}$	respiration of hydrolysis products by fermenters and acetogens	g C m^{-2} h^{-1}	[G1,G2,G3,G6]		
$R_{i,m}$	respiration of acetate by acetotrophic methanogens	g C m^{-2} h^{-1}	[G7,G8,G9,G11]		
$\boldsymbol{R'_m}$	specific respiration by acetotrophic methanogens at saturating [$A_{i,c}$], 30 °C and zero water potential	g C g $M_{i,m,a}^{-1}$ h^{-1}	[G7]	0.20	Smith and Mah (1980)
$R_{\mathrm{m}h,j}$	maintenance respiration by hydrogenotrophic methanogens	g C m^{-2} h^{-1}	[G14,G17]		

$R_{\mathrm{m}i,f,j}$	maintenance respiration by fermenters and acetogens	g C m^{-2} h^{-1}	[G3,G6]
$R_{\mathrm{m}i,m,j}$	maintenance respiration by acetotrophic methanogens	g C m^{-2} h^{-1}	[G9,G11]
$R_{\mathrm{m}t,j}$	maintenance respiration by methanotrophs	g C m^{-2} h^{-1}	[G25,G27]
R_t	CH_4 oxidation by methanotrophs for respiration	g C m^{-2} h^{-1}	[G21b,G23,G24, G25,G27a]
R'_t	CH_4 oxidation by methanotrophs for respiration at saturating O_2	g C m^{-2} 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	g C m^{-2} h^{-1}	[G14,G17,G18]
$U_{i,f,k}$	rate of $DOC_{i,k}$ uptake by $M_{i,f}$	g C m^{-2} h^{-1}	[G3,G6]
$U_{i,m,c}$	rate of $A_{i,c}$ uptake by $M_{i,m}$	g C m^{-2} h^{-1}	[G9,G11]
$U_{t,c}$	rate of CH_4 uptake by M_t	g C m^{-2} h^{-1}	[G25,G27]
X_t	CH_4 oxidation by methanotrophs	g C m^{-2} h^{-1}	[G21a,G22]

X'_t	CH_4 oxidation by methanotrophs at saturating O_2	g C m^{-2} h^{-1}	[G1,G2,G4a]		
$\boldsymbol{X'_t}$	specific CH_4 oxidation by methanotrophs at saturating O_2, 30 °C and zero water potential	g C g^{-1} h^{-1}	[G18]	0.5	Conrad (1984)
Y_f	biomass yield from fermentation and acetogenic reactions	g $M_{i,f}$ g $DOC_{i,c}^{-1}$	[G3,G4]		
Y_h	biomass yield from hydrogenotrophic methanogenic reaction	g M_h g CO_2-C^{-1}	[G14,G15,G18]		
Y_m	biomass yield from acetotrophic methanogenic reaction	g $M_{i,m}$ g $A_{i,c}^{-1}$	[G9,G10]		
Y_{t_G}	biomass yield from methanotrophic growth respiration	g M_t-C g CH_4-C^{-1}	[G25a,G26]		
Y_{t_R}	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 NH_4^+ by all microbial populations

$$I_{\mathrm{NH_4}i,n,j} = (M_{i,m,j,\mathrm{C}}\boldsymbol{C_{\mathrm{N}j}} - M_{i,m,j,\mathrm{N}}) \qquad (I_{\mathrm{NH_4}i,n,j} < 0) \qquad \text{[H1a]}$$

$$I_{\mathrm{NH_4}i,n,j} = (M_{i,m,j,\mathrm{C}}\boldsymbol{C_{\mathrm{N}j}} - M_{i,m,j,\mathrm{N}})[\mathrm{NH_4}^+]/([\mathrm{NH_4}^+] + \boldsymbol{K_{\mathrm{NH_4}m}}) \qquad (I_{\mathrm{NH_4}i,n,j} > 0) \qquad \text{[H1b]}$$

$$I_{\mathrm{NO_3}i,n,j} = (M_{i,m,j,\mathrm{C}}\boldsymbol{C_{\mathrm{N}j}} - (M_{i,m,j,\mathrm{N}} + I_{\mathrm{NH_4}i,n,j}))\ [\mathrm{NO_3}^-]/([\mathrm{NO_3}^-] + K_{\mathrm{NO_3}m}) \qquad (I_{\mathrm{NO_3}i,n,j} > 0) \qquad \text{[H1b]}$$

Oxidation of DOC and reduction of O_2 by heterotrophs

$$X'_{\mathrm{DOC}i,h} = \{X'_{\mathrm{DOC}}\ M_{i,h,a}\ [\mathrm{DOC}_i]/([\mathrm{DOC}_i]) + \boldsymbol{K_{\mathrm{X}h}}\}\ f_{\mathrm{t}} \qquad \text{[H2]}$$

$$R'_{\mathrm{O}_2 i,h} = \mathbf{RQ_C}\, X'_{\mathrm{DOC}i,h} \qquad \text{[H3]}$$

$$R_{\mathrm{O}_2 i,h} = 4\pi n M_{i,h,a} D_{\mathrm{sO}_2}\,([\mathrm{O}_{2\mathrm{s}}] - [\mathrm{O}_{2\mathrm{m}i,h}])[r_\mathrm{m} r_\mathrm{w}/(r_\mathrm{w} - r_\mathrm{m})] \qquad \text{[H4a]}$$

$$= R'_{\mathrm{O}_2 i,h}[\mathrm{O}_{2\mathrm{m}i,h}]/([\mathrm{O}_{2\mathrm{m}i,h}] + \boldsymbol{K}_{\mathbf{O_2}\boldsymbol{h}}) \qquad \text{[H4b]}$$

$$X_{\mathrm{DOC}i,h} = X'_{\mathrm{DOC}i,h}\; R_{\mathrm{O}_2 i,h} / R'_{\mathrm{O}_2 i,h} \qquad \text{[H5]}$$

Oxidation of DOC and reduction of NO_3^-, NO_2^- and N_2O by denitrifiers

$$R'_{\mathrm{NO}_3 i,d} = \boldsymbol{E}_{\mathbf{No_x}}\, \boldsymbol{f}_{\mathbf{e}}\,(R'_{\mathrm{O}_2 i,d} - R_{\mathrm{O}_2 i,d}) \qquad \text{[H6]}$$

$$R_{\mathrm{NO}_3 i,d} = R'_{\mathrm{NO}_3 i,d}\,[\mathrm{NO}_3^-]/([\mathrm{NO}_3^-] + \boldsymbol{K}_{\mathbf{NO_3}\boldsymbol{d}}) \qquad \text{[H7]}$$

$$R_{\mathrm{NO}_2 i,d} = (R'_{\mathrm{NO}_3 i,d} - R_{\mathrm{NO}_3 i,d})\,[\mathrm{NO}_2^-]/([\mathrm{NO}_2^-] + \boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{d}}) \qquad \text{[H8]}$$

$$R_{\mathrm{N}_2\mathrm{O}i,d} = 2\,(R'_{\mathrm{NO}_3 i,d} - R_{\mathrm{NO}_3 i,d} - R_{\mathrm{NO}_2 i,d})\,[\mathrm{N}_2\mathrm{O}]/([\mathrm{N}_2\mathrm{O}] + \boldsymbol{K}_{\mathbf{N_2O}\boldsymbol{d}}) \qquad \text{[H9]}$$

$$X_{\mathrm{DOC}i,d} = X_{\mathrm{DOC}i,d}\ (\text{from [H5]}) + \boldsymbol{F}_{\mathbf{NO_x}}\,(R_{\mathrm{NO}_3 i,d} + R_{\mathrm{NO}_2 i,d}) + \boldsymbol{F}_{\mathbf{N_2O}}\, R_{\mathrm{N}_2\mathrm{O}i,d} \qquad \text{[H10]}$$

Oxidation of NH_3 and reduction of O_2 by nitrifiers

$$X'_{\mathrm{NH}_3 i,n} = X'_{\mathrm{NH}_3}\, M_{\boldsymbol{i,n,a}}\, \{[\mathrm{NH}_{3\mathrm{S}}]/([\mathrm{NH}_{3\mathrm{S}}] + \boldsymbol{K}_{\mathbf{NH_3}\boldsymbol{n}})\}\, \{[\mathrm{CO}_{2\mathrm{S}}]/([\mathrm{CO}_{2\mathrm{S}}] + \boldsymbol{K}_{\mathbf{CO_2}})\}\; f_\mathrm{t} \qquad \text{[H11]}$$

$$R'_{\mathrm{O}_2 i,n} = \mathbf{RQ_{NH_3}}\, X'_{\mathrm{NH}_3 i,n} + \mathbf{RQ_C}\, X'_{\mathrm{C}i,n} \qquad \text{[H12]}$$

$$R_{\mathrm{O}_2 i,n} = 4\pi\, n\, M_{i,n,a}\, D_{\mathrm{sO}_2}\,(r_\mathrm{m}\, r_\mathrm{w}/(r_\mathrm{w} - r_\mathrm{m}))\,([\mathrm{O}_{2\mathrm{S}}] - [\mathrm{O}_{2\mathrm{m}i,n}]) \qquad \text{[H13a]}$$

$$= R'_{\mathrm{O}_2 i,n}\,[\mathrm{O}_{2\mathrm{m}i,n}]/([\mathrm{O}_{2\mathrm{m}i,n}] + \boldsymbol{K}_{\mathbf{O_2}\boldsymbol{n}}) \qquad \text{[H13b]}$$

$$X_{\mathrm{NH}_3 i,n} = X'_{\mathrm{NH}_3 i,n}\, R_{\mathrm{O}_2 i,n} / R'_{\mathrm{O}_2 i,n} \qquad \text{[H14]}$$

Oxidation of NO_2^- and reduction of O_2 by nitrifiers

$$X'_{NO_2 i,o} = X'_{NO_2}\ M_{i,o,a}\ \{[NO_2^-]/([NO_2^-] + \boldsymbol{K_{NO_2 o}})\}\ \{[CO_{2S}]/([CO_{2S}] + \boldsymbol{K_{CO_2}})\}\ f_t \qquad [H15]$$

$$R'_{O_2 i,o} = \mathbf{RQ_{NO_2}}\ X'_{NO_2 i,o} + \mathbf{RQ_C}\ X'_{Ci,o} \qquad [H16]$$

$$R_{O_2 i,o} = 4\pi\ n\ M_{i,o,a}\ D_{sO_2}\ (r_m\ r_w/(r_w - r_m))\ ([O_{2s}] - [O_{2mi,o}]) \qquad [H17a]$$

$$= R'_{O_2 i,o}\ [O_{2mi,o}]/([O_{2mi,o}] + \boldsymbol{K_{O_2 o}}) \qquad [H17b]$$

$$X_{NO_2 i,o} = X'_{NO_2 i,o}\ R_{O_2 i,o} / R'_{O_2 i,o} \qquad [H18]$$

Oxidation of NH_3 and reduction of NO_2^- by nitrifiers

$$R'_{NO_2 i,n} = \boldsymbol{E_{NO_x}}\ \boldsymbol{f_e}\ (R'_{O_2 i,n} - R_{O_2 i,n}) \qquad [H19]$$

$$R_{NO_2 i,n} = R'_{NO_2 i,n}\ \{[NO_2^-]/([NO_2^-] + \boldsymbol{K_{NO_2 n}})\}\{[CO_{2S}]/([CO_{2S}] + \boldsymbol{K_{CO_2}})\} \qquad [H20]$$

$$X_{NH_3 i,n} = X_{NH_3 i,n}\ (\text{from [H14]}) + 0.33\ R_{NO_2 i,n} \qquad [H21]$$

Definition of variables in appendix H

Name	Definition	Units	Equations	Input Values	Reference
	Subscripts				
a	active component of $M_{i,m}$				
d	heterotrophic denitrifier population (subset of *h*)				

h	heterotrophic community (subset of m)
i	substrate-microbe complex
j	kinetic components of $\mathrm{M}_{i,m}$
m	all microbial communities
n	autotrophic ammonia oxidizer population (subset of m)
o	autotrophic nitrite oxidizer population (subset of m)

Variables

$\boldsymbol{C}_{\mathbf{N}\boldsymbol{j}}$	maximum ratio of $M_{i,m,j,\mathrm{N}}$ to $M_{i,m,j,\mathrm{C}}$ maintained by $M_{i,m,j}$	g N g C^{-1}	[H1]	0.22 and 0.13 for j = labile and resistant
$[\mathrm{CO}_{2\mathrm{S}}]$	CO_2 concentration in soil solution	g C m^{-3}	[H11,H15,H20]	
$[\mathrm{DOC}_i]$	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]	
$\boldsymbol{E}_{\mathbf{NO_x}}$	e$^-$ accepted by NO_x vs. O_2 when oxidizing DOC	g N g O_2^{-1}	[H6,H19]	28/32 = 0.875
$\boldsymbol{F}_{\mathbf{NO_x}}$	e$^-$ donated by C vs. e$^-$ accepted by NO_x when oxidizing DOC	g C g N^{-1}	[H10]	12/28 = 0.43

$\boldsymbol{F}_{\mathbf{N_2O}}$	e^- donated by C vs. e^- accepted by N_2O when oxidizing DOC	$g\ C\ g\ N^{-1}$	[H10]	6/28 = 0.215	
$\boldsymbol{f}_{\mathbf{e}}$	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]		
$I_{NH_4 i,n,j}$	mineralization ($I_{NH_4 i,n,j} < 0$) or immobilization ($I_{NH_4 i,n,j} > 0$) of NH_4^+ by $M_{i,n,j,C}$	$g\ N\ m^{-2}\ h^{-1}$	[H1]		
$I_{NO_3 i,n,j}$	immobilization ($I_{NO_3 i,n,j} > 0$) of NO_3^- by $M_{i,n,j,C}$	$g\ N\ m^{-2}\ h^{-1}$	[H1]		
$\boldsymbol{K}_{\mathbf{CO_2}}$	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	
$\boldsymbol{K}_{\mathbf{NH_3}\boldsymbol{n}}$	M-M constant for oxidation of NH_{3S} by nitrifiers	$g\ N\ m^{-3}$	[H11]	0.01	Suzuki et al. (1974)
$\boldsymbol{K}_{\mathbf{NH_4}\boldsymbol{m}}$	M-M constant for microbial NH_4^+ uptake	$g\ N\ m^{-3}$	[H1]	0.35	
$\boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{d}}$	M-M constant for reduction of NO_2^- by denitrifiers	$g\ N\ m^{-3}$	[H8]	3.5	Yoshinari et al. (1977)
$\mathbf{K}_{\mathbf{NO_2}\boldsymbol{n}}$	M-M constant for reduction of NO_2^- by nitrifiers	$g\ N\ m^{-3}$	[H20]	3.5	

$\boldsymbol{K_{\mathrm{NO_2}o}}$	M-M constant for oxidation of NO_2^- by nitrifiers	g N m^{-3}	[H15]	10	
$\boldsymbol{K_{\mathrm{NO_3}d}}$	M-M constant for reduction of NO_3^- by denitrifiers	g N m^{-3}	[H7]	3.5	Yoshinari et al. (1977)
$\boldsymbol{K_{\mathrm{N_2O}d}}$	M-M constant for reduction of N_2O by denitrifiers	g N m^{-3}	[H9]	0.35	Yoshinari et al. (1977)
$\boldsymbol{K_{\mathrm{O_2}h}}$	M-M constant for reduction of O_{2s} by heterotrophs	g O_2 m^{-3}	[H4b]	0.064	Griffin (1972)
$\boldsymbol{K_{\mathrm{O_2}n}}$	M-M constant for reduction of O_{2s} by NH_3 oxidizers	g O_2 m^{-3}	[H13b]	0.32	Focht and Verstraete (1977)
$\boldsymbol{K_{\mathrm{O_2}o}}$	M-M constant for reduction of O_{2s} by NO_2^- oxidizers	g O_2 m^{-3}	[H17b]	0.32	Focht and Verstraete (1977)
$\boldsymbol{K_{\mathrm{X}h}}$	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]		

$M_{i,m,j,\mathrm{C}}$	C biomass of microbial population $M_{i,m,j}$	g C m^{-2}	[H1]
$M_{i,m,j,\mathrm{N}}$	N biomass of microbial population $M_{i,m,j}$	g N m^{-2}	[H1]
$M_{i,o,a}$	active biomass of NO_2^- oxidizers	g C m^{-2}	[H15,H17]
$[NH_{3s}]$	concentration of NH_3 in soil solution	g N m^{-3}	[H11]
$[NH_4^+]$	concentration of NH_4^+ in soil solution	g N m^{-3}	[H1]
$[NO_2^-]$	concentration of NO_2^- in soil solution	g N m^{-3}	[H8,H15,H20]
$[NO_3^-]$	concentration of NO_3^- in soil solution	g N m^{-3}	[H7]
$[N_2O]$	concentration of N_2O in soil solution	g N m^{-3}	[H9]
n	number of microbes	g^{-1}	[H13,H17]
$[O_{2\mathrm{m}i,h}]$	O_2 concentration at heterotrophic surfaces	g O_2 m^{-3}	[H7]
$[O_{2\mathrm{m}i,n}]$	O_2 concentration at NH_3 oxidizer surfaces	g O_2 m^{-3}	[H13]
$[O_{2\mathrm{m}i,o}]$	O_2 concentration at NO_2^- oxidizer surfaces	g O_2 m^{-3}	[H17]
$[O_{2\mathrm{s}}]$	O_2 concentration in soil solution	g O_2 m^{-3}	[H7,H13,H17]
$R_{\mathrm{NO}_2 i,d}$	NO_2^- reduction by denitrifiers	g N m^{-2} h^{-1}	[H8,H9,H10]
$R'_{\mathrm{NO}_2 i,n}$	rate of NO_2^- reduction by NH_3 oxidizers under non-limiting $[NO_2^-]$ and $[CO_{2S}]$	g N m^{-2} h^{-1}	[H19,H20]

$R_{NO_2 i,n}$	rate of NO_2^- reduction by NH_3 oxidizers under ambient $[NO_2^-]$ and $[CO_{2S}]$	$g\ N\ m^{-2}\ h^{-1}$	[H20,H21]
$R'_{NO_3 i,d}$	NO_3^- reduction by denitrifiers under non-limiting $[NO_3^-]$	$g\ N\ m^{-2}\ h^{-1}$	[H6,H7,H8,H9]
$R_{NO_3 i,d}$	NO_3^- reduction by denitrifiers under ambient $[NO_3^-]$	$g\ N\ m^{-2}\ h^{-1}$	[H7,H8,H9,H10]
$R_{N_2O i,d}$	N_2O reduction by denitrifiers	$g\ N\ m^{-2}\ h^{-1}$	[H9,H10]
$R'_{O_2 i,d}$	rate of O_{2S} reduction by denitrifiers under non-limiting $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H6]
$R_{O_2 i,d}$	rate of O_{2S} reduction by denitrifiers under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H6]
$R'_{O_2 i,h}$	rate of O_{2S} reduction by heterotrophs under non-limiting $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H3,H4,H5]
$R_{O_2 i,h}$	rate of O_{2S} reduction by heterotrophs under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H4,H5]
$R'_{O_2 i,n}$	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]

$R_{\mathrm{O}_2 i,n}$	rate of $\mathrm{O}_{2\mathrm{S}}$ reduction by NH_3 oxidizers under ambient [$\mathrm{O}_{2\mathrm{S}}$]	g O_2 m^{-2} h^{-1}	[H13,H14,H19]		
$R'_{\mathrm{O}_2 i,o}$	rate of $\mathrm{O}_{2\mathrm{S}}$ reduction by NO_2^- oxidizers under non-limiting [$\mathrm{O}_{2\mathrm{S}}$]	g O_2 m^{-2} h^{-1}	[H16,H17,H18]		
$R_{\mathrm{O}_2 i,o}$	rate of $\mathrm{O}_{2\mathrm{S}}$ reduction by NO_2^- oxidizers under ambient [$\mathrm{O}_{2\mathrm{S}}$]	g O_2 m^{-2} h^{-1}	[H17,H18]		
$\mathbf{RQ}_{\mathbf{C}}$	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)
$\mathbf{RQ}_{\mathbf{NH_3}}$	respiratory quotient for reduction of O_2 coupled to oxidation of $\mathrm{NH}_{3\mathrm{S}}$	g O_2 g N^{-1}	[H12]	3.43	Brock and Madigan (1991)
$\mathbf{RQ}_{\mathbf{NO_2}}$	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)
$X'_{\mathrm{C}i,n}$	rate of C oxidation by NH_3 oxidizers under non-limiting [$\mathrm{O}_{2\mathrm{S}}$]	g C m^{-2} h^{-1}	[H12]		

$X'_{\mathrm{C}i,o}$	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)
$X'_{\mathrm{DOC}i,h}$	rate of DOC oxidation by heterotrophs under non-limiting [O_{2S}]	g N m^{-2} h^{-1}	[H2,H3,H5]		
$X_{\mathrm{DOC}i,h}$	rate of DOC oxidation by heterotrophs under ambient [O_{2S}]	g N m^{-2} h^{-1}	[H5]		
$X_{\mathrm{DOC}i,d}$	rate of DOC oxidation by heterotrophs under ambient [O_{2S}] and [NO_x]	g N m^{-2} h^{-1}	[H10]		
$X'_{\mathrm{NH_3}}$	specific rate of NH_3 oxidation by NH_3 oxidizers at 25 °C under non-limiting [O_{2S}]	g N g C^{-1} h^{-1}	[H11]]	0.625	Belser and Schmidt (1980)
$X_{\mathrm{NH_3}i,n}$	rate of NH_3 oxidation by NH_3 oxidizers coupled with reduction of O_2 + NO_2^- under ambient [O_{2S}]	g N m^{-2} h^{-1}	[H14,H21]		
$X'_{\mathrm{NH_3}i,n}$	rate of NH_3 oxidation by NH_3 oxidizers under non-limiting [O_{2S}]	g N m^{-2} h^{-1}	[H11,H12,H14]		

$X'_{\mathrm{NO}_2 i,o}$	rate of NO_2^- oxidation by NO_2^- oxidizers under non-limiting [$\mathrm{O}_{2\mathrm{S}}$]	g N m^{-2} h^{-1}	[H15,H16,H18]		
$X_{\mathrm{NO}_2 i,o}$	rate of NO_2^- oxidation by NO_2^- oxidizers coupled with reduction of O_2 under ambient [$\mathrm{O}_{2\mathrm{S}}$]	g N m^{-2} h^{-1}	[H18]		
X'_{NO_2}	specific rate of NO_2^- oxidation by NO_2^- oxidizers at 25 °C under non-limiting [$\mathrm{O}_{2\mathrm{S}}$]	g N g C^{-1} h^{-1}	[H15]	2.5	Belser (1977)

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