Supplement of Biogeosciences, 13, 3549–3571, 2016
http://www.biogeosciences.net/13/3549/2016/
doi:10.5194/bg-13-3549-2016-supplement

Supplement of

Ecological controls on N_2O emission in surface litter and near-surface soil of a managed grassland: modelling and measurements

R. F. Grant et al.

Correspondence to: Robert F. Grant (rgrant@ualberta.ca)

SUPPLEMENTARY MATERIAL

Model Development

General

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

Section A: Soil C, N and P Transformations

Decomposition

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

The rate at which each component of each organic state in each complex is hydrolyzed during decomposition is a first-order function of the decomposer biomass M of all heterotrophic microbial populations [A1]. Decomposer biomasses are redistributed among complexes from active biomasses according to biomass – substrate concentration differences (priming) [A3]. The rate at which each component is hydrolyzed is also a Monod function of substrate concentration [A3, A5], calculated from the fraction of substrate mass colonized by M [A4]. Hydrolysis rates are controlled by T_s through an Arrhenius function [A6] and by soil water content (θ) through its effect on aqueous microbial concentrations [M] [A3, A5] in surface litter and in a spatially resolved soil profile. T_s and θ are calculated from surface energy balances and from heat and water transfer schemes through canopy–snow–residue–soil profiles as described in *Energy*

Exchange above. Release of N and P from hydrolysis of each component in each complex is determined by its N and P concentrations [A7] which are determined from those of the originating litterfall as described in *Autotrophic Respiration and Growth* above. Most non-lignin hydrolysis products are released as dissolved organic C, N and P (DOC, DON, and DOP) which are adsorbed or desorbed according to a power function of their soluble concentrations [A8 – A10].

Microbial Growth

The DOC decomposition product is the substrate for heterotrophic respiration (R_h) by all M in each substrate-microbe complex [A13]. Total R_h for all soil layers [A11] drives CO_2 emission from the soil surface through volatilization and diffusion. R_h may be constrained by microbial N or P concentrations, T_s, DOC and O_2 [A12 - A14]. O_2 uptake by M is driven by R_h [A16] and constrained by O_2 diffusivity to microbial surfaces [A17], as described for roots in *Autotrophic Respiration and Growth* above. Thus R_h is coupled to O_2 reduction by all aerobic M according to O_2 availability. R_h not coupled with O_2 reduction is coupled with the sequential reduction of NO_3^-, NO_2^-, and N_2O by heterotrophic denitrifiers, and with the reduction of organic C by fermenters and acetotrophic methanogens. In addition, autotrophic nitrifiers conduct NH_4^+ and NO_2^- oxidation, and NO_2^- reduction, and autotrophic methanogens and methanotrophs conduct CH_4 production and oxidation.

All microbial populations undergo maintenance respiration $\boldsymbol{R_m}$ [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 decay. M also undergoes first-order decay $\boldsymbol{D_m}$ [A23]. Internal retention and recycling of microbial N and P during decay [A24] is modelled whenever these nutrients constrain R_h [A12]. Changes in M arise from differences between gains from DOC uptake and losses from $\boldsymbol{R_m} + R_g + \boldsymbol{D_m}$ [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 in *Nutrient Uptake and Translocation* above. If immobilization is inadequate to maintain these minimum ratios, then biomass C:N or C:P may rise, but R_h is constrained by N or P present in the lowest concentration with respect to that at the minimum ratio [A12]. Non-symbiotic heterotrophic diazotrophs can also fix aqueous N_2 [A27] to the extent that immobilization is inadequate to maintain their set minimum C:N, but at an additional respiration cost [A28]. Changes in microbial N and P arise from DON and DOP uptake plus NH_4^+, NO_3^-, and $H_2PO_4^-$ immobilization and N_2 fixation, less NH_4^+, NO_3^-, and $H_2PO_4^-$ mineralization and microbial N and P decomposition [A29].

Humification

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

Section C: Gross Primary Productivity, Autotrophic Respiration, Growth and Litterfall

C_3 Gross Primary Productivity

After successful convergence for T_c and ψ_c (described in *Plant Water Relations* above), V_c is recalculated from that under zero ψ_c (V_c') to that under ambient ψ_c. This recalculation is driven by stomatal effects on V_g [C2] from the increase in r_{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* below. 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, 1998). Thus R_c is coupled to O_2 reduction by all root and mycorrhizal populations according to O_2 availability. R_c is first used to meet maintenance respiration requirements (R_m), calculated independently of R_c from the N content in each organ, and a function of T_c or T_s [C16]. Any excess of R_c over R_m is expended as growth respiration R_g, constrained by branch, root or mycorrhizal ψ_t [C17]. When R_m exceeds R_c, the shortfall is met by the respiration of remobilizable C (R_s) in leaves and twigs or roots and mycorrhizae [C15].

Growth and Litterfall

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

The translocation of σ_C, σ_N and σ_P among branches and root and mycorrhizal layers is driven by concentration gradients generated by production of σ_C from branch GPP and of σ_N and σ_P from root and mycorrhizal uptake vs. consumption of σ_C, σ_N and σ_P from R_c, R_g and phytomass growth (Grant 1998). Low 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, C19a,b]. 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 [C19c,d]. This withdrawal drives the withdrawal of associated remobilizable C, and the loss of associated non-remobilizable C, N and P as litterfall. Environmental constraints such as water, heat, nutrient or O_2 stress that reduce σ_C and hence R_c with respect to R_m therefore hasten litterfall. In addition, concentrations of σ_C,σ_N and σ_P in roots and mycorrhizae drive exudation of nonstructural C, N and P to DOC, DON and DOP in soil [C19e-i].

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

Root and Mycorrhizal Nutrient Uptake

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

C_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 [C10]. Leaf surface N density is controlled by leaf structural N:C and P:C ratios calculated during leaf growth from leaf non-structural N:C and P:C ratios arising from root N and P uptake (Grant, 1998) vs. CO_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 Eq. [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 [C45a] is a hyperbolic function of absorbed irradiance and activity of chlorophyll associated with the bundle sheath with a quantum yield based on 3 ATP [C46]. The provision of reductant from the mesophyll to the bundle sheath in NADP-ME species is not explicitly simulated. RuBPc [C47] and chlorophyll [C48] activities are the products of specific activities and concentrations multiplied by set fractions of leaf surface N density, and from functions of C_3 product inhibition (Bowes, 1991; Stitt, 1991) [C49], ψ_c (Eq. A12 from Grant and Flanagan, 2007) and T_c [C10].

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.

Shoot – Root - Mycorrhizal C, N, P Transfer

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

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

Section 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 depth d_t of, and lateral distance L_t to, an external water table.

Surface Heat Flux

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

Gas Flux

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

Solute Flux

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

Section E: Solute Transformations

Precipitation - Dissolution Equilibria

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

Section H: Inorganic N Transformations

Mineralization and Immobilization of Ammonium by All Microbial Populations

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

Oxidation of DOC and Reduction of Oxygen by Heterotrophs

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

1) DOC oxidation under non-limiting O_2 is calculated from active biomass and DOC concentration ([H2]),
2) O_2 reduction under non-limiting O_2 is calculated from 1) using a set respiratory quotient ([H3]),
3) O_2 reduction under ambient O_2 is calculated from radial O_2 diffusion through water films of thickness determined by soil water potential ([H4a]) coupled with active uptake at heterotroph surfaces driven by 2) ([H4b]). O_2 diffusion and active uptake is population-specific, allowing the development of more anaerobic conditions at microbial surfaces associated with more biologically active substrates. O_2 uptake by heterotrophs also accounts for competition with O_2 uptake by nitrifiers, roots and mycorrhizae,
4) DOC oxidation under ambient O_2 is calculated from 2) and 3) ([H5]). The energy yield of DOC oxidation drives the uptake of additional DOC for construction of microbial biomass $M_{i,h}$ according to construction energy costs of each heterotrophic population (Eqs. [7] to [13] in Grant and Pattey, 2003). Energy costs of denitrifiers are slightly larger than those of obligate heterotrophs, placing denitrifiers at a competitive disadvantage for growth and hence DOC oxidation if electron acceptors other than O_2 are not used.

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

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

1) NO_3^- reduction under non-limiting NO_3^- is calculated from a fraction of electrons demanded by DOC oxidation but not accepted by O_2 because of diffusion limitations ([H6]),
2) NO_3^- reduction under ambient NO_3^- is calculated from 1) depending on relative concentrations and affinities of NO_3^- and NO_2^- [([H7]),
3) NO_2^- reduction under ambient NO_2^- is calculated from demand for electrons not met by NO_3^- in 2) [([H8]) depending on relative concentrations and affinities of NO_2^- and N_2O,
4) N_2O reduction under ambient N_2O is calculated from demand for electrons not met by NO_2^- in 3) [([H9]),
5) additional DOC oxidation enabled by NO_x reduction in 2), 3) and 4) is added to that enabled by O_2 reduction from [H5], the energy yield of which drives additional DOC uptake for construction of $M_{i,n}$. This additional uptake offsets the disadvantage incurred by the larger construction energy costs of denitrifiers.

Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers

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

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

Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers

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

Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers

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

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

Section A: Microbial 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]
$M_{i,d,l,\mathrm{C}} = M_{i,a,l,\mathrm{C}} + \boldsymbol{q_m}\ (M_{i,a,l,\mathrm{C}}\ G_{ix,l,\mathrm{C}} - M_{ix,a,l,\mathrm{C}}\ G_{i,l,\mathrm{C}}) / (G_{ix,l,\mathrm{C}} + G_{i,l,\mathrm{C}})$	redistribution of active microbial biomass populations from each	[A3a]
$M_{i,a,l,\mathrm{C}} = \Sigma_n\ M_{i,n,a,l,\mathrm{C}}$	substrate-microbe complex *i* to other substrate-microbe complexes *ix* according to concentration differences (priming)	[A3b]
$D'_{Si,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Sj,\mathrm{C}}\ [S_{i,j,l,\mathrm{C}}]\} / \{[S_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}\ (1.0 + [\Sigma M_{i,d,l,\mathrm{C}}] / \boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$	substrate and water constraint on *D* from colonized litter, POC and	[A4a]
$D'_{Zi,j,l,\mathrm{C}} = \{\boldsymbol{D}_{Zj,\mathrm{C}}\ [Z_{i,j,l,\mathrm{C}}]\} / \{[Z_{i,j,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}\ (1.0 + [M_{i,d,l,\mathrm{C}}] / \boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$	humus, microbial residues and adsorbed SOC	[A4b]
$D'_{Ai,l,\mathrm{C}} = \{\boldsymbol{D}_{A,\mathrm{C}}\ [A_{i,l,\mathrm{C}}]\} / \{[A_{i,l,\mathrm{C}}] + \boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}\ (1.0 + [M_{i,d,l,\mathrm{C}}] / \boldsymbol{K}_{\mathbf{i}\boldsymbol{D}})\}$		[A4c]
$\delta S_{i,j,k,l,\mathrm{C}} / \delta t = \boldsymbol{\beta}\ \Sigma_n\ (U_{i,n,l\mathrm{C}} - R_{\mathrm{h}i,n,l})\ (S'_{i,j,k,l,\mathrm{C}} / S'_{i,j,l,\mathrm{C}})\ \{(S'_{i,j,l,\mathrm{C}} / S_{i,j,l,\mathrm{C}}) / (S'_{i,j,l,\mathrm{C}} / S_{i,j,l,\mathrm{C}} + \boldsymbol{K}_{\mathbf{i}\boldsymbol{S}})\}$	colonized litter increases with microbial growth into uncolonized litter	[A5]
$f_{\mathrm{tg}l} = T_{\mathrm{s}l}\ \{e^{[B - \boldsymbol{H}_{\mathbf{a}} / (\boldsymbol{R}\ T_{\mathrm{s}l})]}\} / \{1 + e^{[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{s}l}) / (\boldsymbol{R}\ T_{\mathrm{s}l})]} + e^{[(\boldsymbol{S}T_{\mathrm{s}l} - \boldsymbol{H}_{\mathbf{dh}}) / (\boldsymbol{R}\ T_{\mathrm{s}l})]}\}$	Arrhenius function for *D* and R_{h}	[A6]

$D_{Si,j,l,\mathrm{N,P}} = D_{Si,j,l,\mathrm{C}} (S_{i,j,l,\mathrm{N,P}} / S_{i,j,l,\mathrm{C}})$	decomposition of N and P are driven by that of C in litter, POC, humus, microbial residues and adsorbed SOC	[A7a]
$D_{Zi,j,l,\mathrm{N,P}} = D_{Zi,j,l,\mathrm{C}} (Z_{i,j,l,\mathrm{N,P}} / Z_{i,j,l,\mathrm{C}})$		[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

$R_\mathrm{h} = \Sigma_i \Sigma_n \Sigma_l R_{\mathrm{h}i,n,l}$	total heterotrophic respiration	[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, T_s and ψ	[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]
$f_{\psi\mathrm{g}l} = e^{(\sigma\psi_{\mathrm{s}\,l})}$	ψ_s constraints on microbial growth	[A15]
$U'_{\mathrm{O2}i,n,l} = 2.67 R'_{\mathrm{h}\,i,n,l}$	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]
$R_{\mathrm{m}i,n,j,l} = \boldsymbol{R}_\mathrm{m} M_{i,n,j,l,\mathrm{N}} f_{\mathrm{tm}l}$	maintenanace respiration	[A18]
$f_{\mathrm{tm}l} = e^{[\boldsymbol{y} (T_{\mathrm{s}l} - 298.16)]}$	temperature sensitivity of R_m	[A19]
$R_{\mathrm{g}i,n,l} = R_{\mathrm{h}i,n,l} - \Sigma_j R_{\mathrm{m}i,n,j,l}$	growth respiration	[A20]
$U_{i,n,l\mathrm{C}} = \min (R_{\mathrm{h}i,n,l} , \Sigma_j R_{\mathrm{m}i,n,j,l}) + R_{\mathrm{g}i,n,l} (1 + \boldsymbol{\Delta G}_{\boldsymbol{x}} / \boldsymbol{E}_\mathbf{m})$	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]
$D_{Mi,n,j,l,\mathrm{C}} = \boldsymbol{D}_{Mi,j}\, M_{i,n,j,\mathrm{C}}$	first-order decay of microbial C,		[A23]
$D_{Mi,n,j,\mathrm{N,P}} = \boldsymbol{D}_{Mi,j}\, M_{i,n,j,l,\mathrm{N,P}}\, f_{\mathrm{d}i,n,l\mathrm{N,P}}$	decay of microbial N, P		[A24]
$\delta M_{i,n,j,l,\mathrm{C}} / \delta t = F_j\, U_{i,n,l\mathrm{C}} - F_j\, R_{\mathrm{h}i,n,l} - D_{Mi,n,j,l,\mathrm{C}}$	$[R_{\mathrm{h}i,n,l} > R_{\mathrm{m}i,n,j,l}]$	microbial growth	[A25a]
$\delta M_{i,n,j,l,\mathrm{C}} / \delta t = F_j\, U_{i,n,l\mathrm{C}} - R_{\mathrm{m}i,n,j,l} - D_{Mi,n,j,l,\mathrm{C}}$	$[R_{\mathrm{h}i,n,l} < R_{\mathrm{m}i,n,j,l}]$	microbial senescence	[A25b]

Microbial Nutrient Exchange

$U_{\mathrm{NH4}i,n,j,l} = (M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - M_{i,n,j,l,N})$	$U_{\mathrm{NH_4}} < 0$	net mineralization	[A26a]
$U_{\mathrm{NH_4}i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - M_{i,n,j,l,N}),\quad \boldsymbol{U'}_{\mathbf{NH_4}}\, a_{i,n,j,l}\, ([\mathrm{NH_4^+}_{i,n,j,l}] - [\mathbf{NH_4^+}_{\mathbf{mn}}]) / ([\mathrm{NH_4^+}_{i,n,j,l}] - [\mathbf{NH_4^+}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\}$	$U_{\mathrm{NH_4}} > 0$	net immobilization	[A26b]
$U_{\mathrm{NO_3}i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{N}\boldsymbol{j}} - (M_{i,n,j,l,N} + U_{\mathrm{NH_4}i,n,j,l})),\quad \boldsymbol{U'}_{\mathbf{NO_3}}\, a_{i,n,j,l}\, ([\mathrm{NO_3^-}_{i,n,j,l}] - [\mathbf{NO_3^-}_{\mathbf{mn}}]) / ([\mathrm{NO_3^-}_{i,n,j,l}] - [\mathbf{NO_3^-}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\}$	$U_{\mathrm{NO_3}} > 0$	net immobilization	[A26c]
$U_{\mathrm{PO4}i,n,j,l} = (M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{P}\boldsymbol{j}} - M_{i,n,j,l,P})$	$U_{\mathrm{PO_4}} < 0$	net mineralization	[A26d]
$U_{\mathrm{PO4}i,n,j,l} = \min\{(M_{i,n,j,l,C}\ \boldsymbol{C}_{\mathbf{P}\boldsymbol{j}} - M_{i,n,j,l,P}),\quad \boldsymbol{U'}_{\mathbf{PO_4}}\, A_{i,n,j,l}\, ([\mathrm{H_2PO_4^-}_{i,n,j,l}] - [\mathbf{H_2PO_4^-}_{\mathbf{mn}}]) / ([\mathrm{H_2PO_4^-}_{i,n,j,l}] - [\mathbf{H_2PO_4^-}_{\mathbf{mn}}] + \boldsymbol{K}_{\mathbf{PO_4}})\}$	$U_{\mathrm{PO_4}} > 0$	net immobilization	[A26e]
$\Phi_{i,n=f,j,l} = max\,\{0, M_{i,n=f,j,l,\mathrm{C}}\, \boldsymbol{C}_{\mathrm{N}j} - M_{i,n=f,j,l,\mathrm{N}} - max\{0, U_{i,n=f,j,l,\mathrm{N}}\}\}$	N_2 fixation driven by N deficit of diazotrophic population		[A27]
$R_{\Phi i,n=f,j,l} = \boldsymbol{E}_{\boldsymbol{\Phi}}\, \Phi_{i,n=f,j,l}$	respiration needed to drive N_2 fixation		[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]
$M_{i,n,a,l,\mathrm{C}} = M_{i,n,j=labile,l,\mathrm{C}} + M_{i,n,j=resistant,l,\mathrm{C}}\, F_{\mathrm{r}} / F_{\mathrm{l}}$	active microbial biomass calculated from labile fraction		[A30a]

Humification

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

Definition of Variables in Section 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]	26.235	
$\boldsymbol{b}$	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)
$D_{Ai,l,\mathrm{C}}$	decomposition rate of $A_{i,l,\mathrm{C}}$ by $M_{\boldsymbol{i,d,l},\mathrm{C}}$ 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 $M_{\boldsymbol{i,d,l},\mathrm{C}}$ 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 $M_{\boldsymbol{i,d,l},\mathrm{C}}$	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]		
$\boldsymbol{D}_{Mi,j}$	specific decomposition rate of $M_{i,n,j}$ at 30°C	g C g C^{-1} h^{-1}	[A23,A24]	1.6 x 10^{-3} and 8.0 x 10^{-5} for j = labile and resistant, respectively	Grant et al. (1993a,b)
$D_{Mi,n,j,l,\mathrm{C}}$	decomposition rate of $M_{i,n,j,l,\mathrm{C}}$	g C m^{-2} h^{-1}	[A23,A25,A35,A38]		
$D_{Mi,n,j,l,\mathrm{N,P}}$	decomposition rate of $M_{i,n,j,l,\mathrm{N,P}}$	g N or P m^{-2} h^{-1}	[A24,A29,A39]		
$D_{Si,j,l,\mathrm{C}}$	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, 0.009 for POC, and 0.009 and 0.003 for active and passive humus.	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_{sO2l}	aqueous dispersivity–diffusivity of O2 during microbial uptake in soil	m^{2} h^{-1}	[A17]		
$D_{Zi,j,l,\mathrm{C}}$	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]		
$\boldsymbol{\Delta G_x}$	energy yield of C oxidation with different reductants x	kJ g C^{-1}	[A21]	37.5 (x = O_2), 4.43 (x = DOC)	
$\boldsymbol{E}_{\mathbf{m}}$	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)
F_{clay}	fraction of mineral soil as clay	Mg Mg^{-1}	[A37]		
$\boldsymbol{F}_{\mathbf{h}}$	fraction of products from microbial decomposition that are humified (function of clay content)		[A35, A37]		Sørenson (1981)
$\boldsymbol{F}_{\mathbf{l}}$	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]		

$f_{\mathrm{tm}l}$	temperature function for maintenance respiration	dimensionless	[A18,A19]		
$f_{\psi \mathrm{g}l}$	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, A37]		
$[H_2PO_4^{-}]$	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]	195 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,A38]		
$H_{Mi,n,j,l,\mathrm{N,P}}$	transfer of microbial N or P decomposition products to humus	g N or P m^{-2} h^{-1}	[A36,A39]		
$H_{Si,j,l,\mathrm{C}}$	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]		
$H_{Zi,n,j,l,\mathrm{C}}$	transfer of microbial C decomposition products to microbial residue	g C m m^{-2} h^{-1}	[A38]		
$H_{Zi,n,j,l,\mathrm{N,P}}$	transfer of microbial N or P decomposition products to microbial residue	g N or P m^{-2} h^{-1}	[A39]		
$\boldsymbol{K}_{\boldsymbol{iS}}$	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	
$\boldsymbol{K}_{\mathbf{PO_4}}$	M-M constant for $H_2PO_4^{-}$ uptake at microbial surfaces	g P m^{-3}	[A26]	0.125	
$\boldsymbol{K}_{\mathbf{i}\boldsymbol{D}}$	inhibition constant for $[M_{i,n,a}]$ on $S_{i,\mathrm{C}}$, $Z_{i,\mathrm{C}}$	g C m^{-3}	[A4]	25	Grant et al.

$\boldsymbol{K}_{\mathbf{m}\boldsymbol{D}}$	Michaelis–Menten constant for $D_{Si,j,\mathrm{C}}$	g C Mg^{-1}	[A4]	75	(1993a,b); Lizama and Suzuki (1990)
$\boldsymbol{K}_{\mathbf{m}\boldsymbol{Q}_\mathbf{C}}$	Michaelis–Menten constant for $R'_{\mathrm{h}i,n}$ on $[Q_{i,\mathrm{C}}]$	g C m^{-3}	[A13]	36	
$\boldsymbol{K}_{\mathbf{O_2}}$	Michaelis–Menten constant for reduction of $\mathrm{O}_{2\mathrm{s}}$ by microbes, roots and mycorrhizae	g O_2 m^{-3}	[A17]	0.32	Griffin (1972)
$\boldsymbol{k}_{\mathbf{ts}}$	equilibrium rate constant for sorption	h^{-1}	[A8]	0.01	Grant et al. (1993a,b)
$\boldsymbol{L}_{\mathbf{h}\boldsymbol{j}}$	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	
$\boldsymbol{M}_{\boldsymbol{i,d,l,C}}$	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]		
n	number of microbial microsites	m^{-2}	[A17b]		
$[\mathrm{NH_4}^+{}_{i,n,j,l}]$	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 NO_3^- at microbial surfaces below which $U_{NO_3} = 0$	g N m^{-3}	[A26]	0.03	
$[H_2PO_4^-{}_{i,n,j,l}]$	concentration of $H_2PO_4^-$ at microbial surfaces	g N m^{-3}	[A26]		
$[\mathbf{H_2PO_4^-}_{\mathbf{mn}}]$	concentration of $H_2PO_4^-$ at microbial surfaces below which $U_{PO_4} = 0$	g N m^{-3}	[A26]	0.002	
$[O_{2\mathrm{m}i,n,l}]$	O_2 concentration at heterotrophic microsites	g O_2 m^{-3}	[A17]		
$[O_{2\mathrm{s}l}]$	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]		
$\boldsymbol{q_m}$	rate constant for reallocating $M_{i,a,l,\mathrm{C}}$ to $M_{i,d,l,\mathrm{C}}$	h^{-1}	[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]		
σ	shape parameter in $f_{\psi g}$	-	[A15]	0.2	Choudhury et al., (2011)
$r_{\mathrm{w}l}$	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]		
$\boldsymbol{S'_{i,j,l,C}}$	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]		
$\boldsymbol{U'}_{\mathbf{NH_4}}$	maximum $U_{\mathrm{NH_4}}$ at 25 $^{\mathrm{o}}$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]		
$\boldsymbol{U'}_{\mathbf{NO_3}}$	maximum $U_{\mathrm{NO_3}}$ at 25 $^{\mathrm{o}}$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]	
$\boldsymbol{U'}_{\mathbf{PO_4}}$	maximum $U_{\mathrm{PO_4}}$ at 25 °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 m^{-2} h^{-1}	[A8,A9,A10]	
$Y_{i,l,\mathrm{N,P}}$	sorption of N or P hydrolysis products	g P m^{-2} 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]	

Section C: Gross Primary Productivity, Autotrophic Respiration, Growth and Litterfall

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]
$V_{\mathrm{b}i,j,k,l,m,n,o} = V_{\mathrm{bmax}i,j,k} (C_{\mathrm{c}i,j,k,l,m,n,o} - \mathit{\Gamma}_{i,j,k}) / (C_{\mathrm{c}i,j,k,l,m,n,o}) + K_{\mathrm{c}_i})\ f_{\psi\ i,j,k,l,m,n,o}$	CO$_2$ and water f_ψ constraints on V_b	[C6a]
$V_{\mathrm{bmax}_{i,j,k}} = \boldsymbol{V}_{\mathbf{b}}{}'_{i} \boldsymbol{F}_{\mathbf{rubisco}_i} M_{\mathbf{L}_{\boldsymbol{i,j,k,prot}}} / A_{i,j,k}\ f_{\mathrm{tb}\boldsymbol{i}}\ f_{\mathrm{iC}\boldsymbol{i}}$	temperature f_tb and nutrient f_iC constraints on V_bmax	[C6b]
$\mathit{\Gamma}_{i,j,k} = 0.5\, O_\mathrm{c}\, V_{\mathrm{omax}_{i,j,k}}\ \boldsymbol{K}_{\mathbf{c}_i} / (V_{\mathrm{bmax}_{i,j,k}}\ \boldsymbol{K}_{\mathbf{o}_i})$	CO$_2$ compensation point	[C6c]
$V_{\mathrm{omax}_{i,j,k}} = \boldsymbol{V}_{\mathbf{o}}{}'_{i} \boldsymbol{F}_{\mathbf{rubisco}_i} M_{\mathbf{L}_{\boldsymbol{i,j,k,prot}}} / A_{i,j,k}\ f_{\mathrm{to}\boldsymbol{i}}$	oxygenation	[C6d]
$K_{\mathrm{c}_i} = \boldsymbol{K}_{\mathbf{c}_i}\ f_{\mathrm{tkc}i} (1 + O_\mathrm{c} / (\boldsymbol{K}_{\mathbf{o}_i}\ f_{\mathrm{tko}i}))$	M-M constant for V_b	[C6e]
$V_{\mathrm{j}i,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o}\ Y_{i,j,k,l,m,n,o}\ f_{\psi\ i,j,k,l,m,n,o}$	water constraints on V_j	[C7a]
$Y_{i,j,k,l,m,n,o} = (C_{\mathrm{c}i,j,k,l,m,n,o} - \mathit{\Gamma}_{i,j,k}) / (4.5\ C_{\mathrm{c}i,j,k,l,m,n,o} + 10.5\ \mathit{\Gamma}_{i,j,k})$	carboxylation efficiency of V_j	[C7b]
$J_{i,j,k,l,m,n,o} = (\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k} - ((\boldsymbol{\varepsilon}\, I_{i,l,m,n,o} + J_{\mathrm{max}i,j,k})^2 - 4\boldsymbol{\alpha\varepsilon}\, I_{i,l,m,n,o}\ J_{\mathrm{max}i,j,k})^{0.5}) / (2\boldsymbol{\alpha})$	irradiance constraints on J	[C8a]
$J_{\mathrm{max}i,j,k} = \boldsymbol{V}_{\mathbf{j}}{}'_{i}\ \boldsymbol{F}_{\mathbf{chlorophyll}_i}\ M_{\mathrm{L}_{i,j,k,prot}} / A_{i,j,k}\ f_{\mathrm{tj}i}\ f_{\mathrm{iC}i}$	temperature and nutrient constraints on J_max	[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]

Arrhenius functions for carboxylation, oxygenation and electron transport temperature sensitivity of $\boldsymbol{K}_{\mathbf{c}_i}$, $\boldsymbol{K}_{\mathbf{o}_i}$

$$f_{\mathrm{tb}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}} / (\boldsymbol{R}T_{\mathrm{c}i})] / \{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i}) / (\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}}) / (\boldsymbol{R}T_{\mathrm{c}i})]\} \tag{C10a}$$

$$f_{\mathrm{to}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{o}} - \boldsymbol{H}_{\mathbf{ao}} / (\boldsymbol{R}T_{\mathrm{c}i})] / \{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i}) / (\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}}) / (\boldsymbol{R}T_{\mathrm{c}i})]] \tag{C10b}$$

$$f_{\mathrm{tj}\boldsymbol{i}} = \exp[\boldsymbol{B}_{\mathbf{j}} - \boldsymbol{H}_{\mathbf{aj}} / (\boldsymbol{R}T_{\mathrm{c}i})] / \{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i}) / (\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}}) / (\boldsymbol{R}T_{\mathrm{c}i})]\} \tag{C10c}$$

$$f_{\mathrm{tkc}i} = \exp[\boldsymbol{B}_{\mathbf{kc}} - \boldsymbol{H}_{\mathbf{akc}} / (\boldsymbol{R}T_{\mathrm{c}i})] \tag{C10d}$$

$$f_{\mathrm{tko}i} = \exp[\boldsymbol{B}_{\mathbf{ko}} - \boldsymbol{H}_{\mathbf{ako}} / (\boldsymbol{R}T_{\mathrm{c}i})] \tag{C10e}$$

control of σ_{N} and σ_{P} *vs.* σ_{C} in shoots on V_{b}, V_{j} through product inhibition and on leaf protein growth through leaf structural C:N:P ratios

$$f_{\mathrm{iC}\boldsymbol{i}} = min\{\sigma_{\mathrm{N}i,j} / (\sigma_{\mathrm{N}i,j} + \sigma_{\mathrm{C}i,j} / \boldsymbol{K}_{\mathbf{iC_N}}), \sigma_{\mathrm{P}i,j} / (\sigma_{\mathrm{P}i,j} + \sigma_{\mathrm{C}i,j} / \boldsymbol{K}_{\mathbf{iC_P}})\} \tag{C11}$$

growth of remobilizable leaf protein C

$$\delta M_{\mathrm{L_R}i,j,k} / \delta t = \delta M_{\mathrm{L}_{i,j,k}} / \delta t \min\{[\boldsymbol{N'}_{\mathbf{leaf}} + (\boldsymbol{N}_{\mathbf{leaf}} - \boldsymbol{N'}_{\mathbf{leaf}}) f_{\mathrm{iC}\boldsymbol{i}}] / \mathbf{N}_{\mathbf{prot}}, [\boldsymbol{P'}_{\mathbf{leaf}} + (\boldsymbol{P}_{\mathbf{leaf}} - \boldsymbol{P'}_{\mathbf{leaf}}) f_{\mathrm{iC}\boldsymbol{i}}] / \mathrm{P}_{\mathrm{prot}}\} \tag{C12}$$

Autotrophic Respiration

total autotrophic respiration

$$R_{\mathrm{a}} = \Sigma_i \Sigma_{,j} (R_{\mathrm{c}i,j} + R_{\mathrm{s}i,j}) + \Sigma_i \Sigma_l \Sigma_z (R_{\mathrm{c}i,r,l} + R_{\mathrm{s}i,r,l}) + \boldsymbol{E}_{\mathbf{N,P}} (U_{\mathrm{NH4}i,r,l} + U_{\mathrm{NO3}i,r,l} + U_{\mathrm{PO4}i,r,l}) \tag{C13}$$

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

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

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

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

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

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

$R_{\mathrm{s}i,j} = -\,\mathit{min}\{0.0,\ R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j}\}$	remobilization in branchs, roots and mycorrhizae when $R_\mathrm{m} > R_\mathrm{c}$	[C15]
$R_{\mathrm{s}i,r,l} = -\,\mathit{min}\{0.0,\ R_{\mathrm{c}i,r,l} - R_{\mathrm{m}i,r,l}\}$		
$R_{\mathrm{m}i,j} = \Sigma_z\,(\mathrm{N}_{i,j,z}\ \boldsymbol{R}_{\mathbf{m}}'\ f_{\mathrm{tm}i})$	maintenance respiration of branchs, roots and mycorrhizae	[C16]
$R_{\mathrm{m}i,r,l} = \Sigma_z\,(\mathrm{N}_{i,r,l,z}\ \boldsymbol{R}_{\mathbf{m}}'\ f_{\mathrm{tm}i})$		
$R_{\mathrm{g}i,j} = \mathit{max}\{0.0,\ \mathit{min}\{(R_{\mathrm{c}i,j} - R_{\mathrm{m}i,j})\ \mathit{min}\{1.0,\ \mathit{max}\{0.0,\ \psi_{ti} - \psi_\mathrm{t}'\}\}$	growth respiration of branchs, roots and mycorrhizae when $R_\mathrm{m} < R_\mathrm{c}$	[C17]
$R_{\mathrm{g}i,r,l} = \mathit{max}\{0.0,\ \mathit{min}\{(R_{\mathrm{c}i,r,l} - R_{\mathrm{m}i,r,l})\ \mathit{min}\{1.0,\ \mathit{max}\{0.0,\ \psi_{\mathrm{t}i,l} - \psi_\mathrm{t}'\}\}$		

Growth and Litterfall

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

$\delta M_{\mathrm{B}i,j}/\delta t = \Sigma_z\,[R_{\mathrm{g}i,j}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,z})/\boldsymbol{Y}_{\mathbf{g}i,z}] - R_{\mathrm{s}i,j} - l_{i,j,\mathrm{C}}$	branch growth driven by R_{g}	[C20a]
$\delta M_{\mathrm{R}i,r,l}/\delta t = [R_{\mathrm{g}i,r,l}\,(1 - \boldsymbol{Y}_{\mathbf{g}i,r})/\boldsymbol{Y}_{\mathbf{g}i,r}] - R_{\mathrm{s}i,r,l} - l_{i,r,l,\mathrm{C}}$	root growth driven by R_{g}	[C20b]
$\delta A_{\mathrm{L}i,j,k,l}/\delta t = \boldsymbol{\chi}\,(M_{\mathrm{L}i,j,k,l}/y_i)^{-0.33}\,\delta M_{\mathrm{L}i,j,k,l}/\delta t\,\min\{1, \max\{0, \psi_{\mathrm{t}i} - \psi_{\mathrm{t}}'\}$	leaf expansion driven by leaf mass growth	[C21a]
$\delta L_{i,r,l,1}/\delta t = (\delta M_{\mathrm{R}i,r,l,1}/\delta t)/y_i\,\nu_r/\{\rho_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r})\,(\pi\, r_{\mathrm{r}i,r,l,1}{}^{2})\}$	root extension of primary and secondary axes driven by root mass growth	[C21b]
$\delta L_{i,r,l,2}/\delta t = (\delta M_{\mathrm{R}i,r,l,2}/\delta t)\,\nu_r/\{\rho_r\,(1 - \boldsymbol{\theta}_{\mathbf{P}i,r})\,(\pi\, r_{\mathrm{r}i,r,l,2}{}^{2})\}$		[C21c]
$f_{\mathrm{ta}i} = T_{\mathrm{c}i}\{\exp[\boldsymbol{B}_{\mathbf{v}} - \boldsymbol{H}_{\mathbf{av}}/(\boldsymbol{R}T_{\mathrm{c}i})]\}/\{1 + \exp[(\boldsymbol{H}_{\mathbf{dl}} - \boldsymbol{S}T_{\mathrm{c}i})/(\boldsymbol{R}T_{\mathrm{c}i})] + \exp[(\boldsymbol{S}T_{\mathrm{c}i} - \boldsymbol{H}_{\mathbf{dh}})/(\boldsymbol{R}T_{\mathrm{c}i})]\}$	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

$U_{\mathrm{NH4}i,r,l} = \{U_{\mathrm{w}i,r,l}[\mathrm{NH}_4{}^{+}{}_{l}] + 2\pi L_{i,r,l}D_{\mathrm{eNH}_4 l}\,([\mathrm{NH}_4{}^{+}{}_{l}] - [\mathrm{NH}_4{}^{+}{}_{i,r,l}])/\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\}$	root N and P uptake from mass flow + diffusion coupled with active uptake of $\mathrm{NH}_4{}^{+}$, $\mathrm{NO}_3{}^{-}$ and $\mathrm{H}_2\mathrm{PO}_4{}^{-}$ constrained by O_2 uptake, as modelled for microbial N and P uptake in [A26]	[C23a]
$= \boldsymbol{U}'_{\mathbf{NH_4}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{NH}_4{}^{+}{}_{i,r,l}] - [\mathbf{NH_4{}^{+}{}_{mn}}])/([\mathrm{NH}_4{}^{+}{}_{i,r,l}] - [\mathbf{NH_4{}^{+}{}_{mn}}] + \boldsymbol{K}_{\mathbf{NH_4}})\,f_{\mathrm{ta}i,l}\,f_{\mathrm{iN}i,r,l}$		[C23b]
$U_{\mathrm{NO3}i,r,l} = \{U_{\mathrm{w}i,r,l}\,[\mathrm{NO}_3{}^{-}{}_{l}] + 2\pi L_{i,r,l}\,D_{\mathrm{eNO}_3 l}\,([\mathrm{NO}_3{}^{-}{}_{l}] - [\mathrm{NO}_3{}^{-}{}_{i,r,l}])/\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\}$		[C23c]
$= \boldsymbol{U}'_{\mathbf{NO_3}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{NO}_3{}^{-}{}_{i,r,l}] - [\mathbf{NO_3{}^{-}{}_{mn}}])/([\mathrm{NO}_3{}^{-}{}_{i,r,l}] - [\mathbf{NO_3{}^{-}{}_{mn}}] + \boldsymbol{K}_{\mathbf{NO_3}})\,f_{\mathrm{ta}i,l}\,f_{\mathrm{iN}i,r,l}$		[C23d]
$U_{\mathrm{PO4}i,r,l} = \{U_{\mathrm{w}i,r,l}\,[\mathrm{H}_2\mathrm{PO}_4{}^{-}{}_{l}] + 2\pi L_{i,r,l}D_{\mathrm{ePO}_4 l}\,([\mathrm{H}_2\mathrm{PO}_4{}^{-}{}_{l}] - [\mathrm{H}_2\mathrm{PO}_4{}^{-}{}_{i,r,l}])/\ln(d_{i,r,l}/r_{\mathrm{r}i,r,l})\}$		[C23e]
$= \boldsymbol{U}'_{\mathbf{PO_4}}\,(U_{\mathrm{O2}i,r,l}/U'_{\mathrm{O2}i,r,l})\,A_{i,r,l}\,([\mathrm{H}_2\mathrm{PO}_4{}^{-}{}_{i,r,l}] - [\mathbf{H_2PO_4{}^{-}{}_{mn}}])/([\mathrm{H}_2\mathrm{PO}_4{}^{-}{}_{i,r,l}] - [\mathbf{H_2PO_4{}^{-}{}_{mn}}] + \boldsymbol{K}_{\mathbf{PO_4}})\,f_{\mathrm{ta}i,l}\,f_{\mathrm{iP}i,r,l}$		[C23f]
$f_{\mathrm{iN}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{N}i,r,l}/\boldsymbol{K}_{\mathbf{iN_C}})$	product inhibition of U_{NH4}, U_{NO3} and U_{PO4} determined by σ_{N} and σ_{P} *vs.* σ_{C} in roots	[C23g]
$f_{\mathrm{iP}i,r,l} = \sigma_{\mathrm{C}i,r,l}/(\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{P}i,r,l}/\boldsymbol{K}_{\mathbf{iP_C}})$		[C23h]

C_4 Gross Primary Productivity

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 [C30a]

$Y_{\mathrm{(m4)}i,j,k} = (C_{\mathrm{c(m4)}i,j,k,l,m,n,o} - \Gamma_{\mathrm{(m4)}i,j,k}) / (3.0\ C_{\mathrm{c(m4)}i,j,k,l,m,n,o}) + 10.5\ \Gamma_{\mathrm{(m4)}i,j,k})$ [C30b]

$J_{\mathrm{(m4)}i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(m4)}i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(m4)}i,j,k})^2 - 4\alpha\varepsilon I_{i,l,m,n,o} J_{\mathrm{max(m4)}i,j,k})^{0.5}) / (2\alpha)$ irradiance response function [C31]

$V_{\mathrm{bmax(m4)}i,j,k} = V_{\mathrm{bmax(m4)}}' [N_{\mathrm{pep(m4)}i,j,k}]'\ N_{\mathrm{lf}i,j,k}\ A_{\mathrm{lf}i,j,k}\ f_{\mathrm{C(m4)}i,j,k} f_{\psi i}\ f_{\mathrm{tb}i}$ PEPc activity [C32]

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

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]

$V_{\phi\mathrm{(b4)}i,j,k} = \kappa_{\mathrm{Cc(b4)}} (C_{\mathrm{c(b4)}i,j,k} - C_{\mathrm{c(m4)}i,j,k}) (12 \times 10^{-9})\ W_{\mathrm{lf(b4)}i,j,k}$ 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	[C45a]
$Y_{\mathrm{(b4)}i,j,k} = (C_{\mathrm{c(b4)}i,j,k} - \Gamma_{\mathrm{(b4)}i,j,k}) / (4.5\ C_{\mathrm{c(b4)}i,j,k} + 10.5\ \Gamma_{\mathrm{(b4)}i,j,k})$	carboxylation efficiency of $V_{\mathrm{j(b4)}}$	[C45b]
$J_{\mathrm{(b4)}i,j,k,l,m,n,o} = (\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(b4)}i,j,k} - ((\varepsilon I_{i,l,m,n,o} + J_{\mathrm{max(b4)}i,j,k})^2 - 4\alpha\varepsilon\ I_{i,l,m,n,o} J_{\mathrm{max(b4)}i,j,k})^{0.5}) / (2\alpha)$	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]

Shoot – Root - Mycorrhizal C, N, P Transfer

$Z_{s\mathrm{C}i,j\text{-}i,r,l} = g_{s\mathrm{C}i,j\text{-}i,r,l}\ (\sigma_{\mathrm{C}i,j}\ M_{\mathrm{R}i,r,l} - \sigma_{\mathrm{C}i,r,l}\ M_{\mathrm{B}i,j}) / (M_{\mathrm{R}i,r,l} + M_{\mathrm{B}i,j})$	shoot – root C transfer driven by σ_{C} concentration gradients	[C50]
$Z_{s\mathrm{N,P}i,j\text{-}i,r,l} = \boldsymbol{g}_{\boldsymbol{s}\mathbf{N,P}i,j\text{-}i,r,l}\ (\sigma_{\mathrm{N,P}i,j}\ \sigma_{\mathrm{C}i,r,l} - \sigma_{\mathrm{N,P}i,r,l}\ \sigma_{\mathrm{C}i,j}) / (\sigma_{\mathrm{C}i,r,l} + \sigma_{\mathrm{C}i,j})$	shoot – root N,P transfer driven by $\sigma_{\mathrm{N,P}}$ concentration gradients	[C51]
$Z_{r\mathrm{C}i,j\text{-}i,r,l} = \boldsymbol{g}_{\boldsymbol{r}\mathbf{C}i,j\text{-}i,r,l}\ (\sigma_{\mathrm{C}i,r,l}\ M_{\mathrm{M}i,r,l} - \sigma_{\mathrm{C}i,m,l}\ M_{\mathrm{R}i,r,l}) / (M_{\mathrm{M}i,r,l} + M_{\mathrm{R}i,r,l})$	root – mycorrhizal C transfer driven by σ_{C} conc’n gradients	[C52]
$Z_{r\mathrm{N,P}i,j\text{-}i,r,l} = \boldsymbol{g}_{\boldsymbol{r}\mathbf{N,P}i,j\text{-}i,r,l}\ (\sigma_{\mathrm{N,P}i,r,l}\ \sigma_{\mathrm{C}i,m,l} - \sigma_{\mathrm{N,P}i,m,l}\ \sigma_{\mathrm{C}i,r,l}) / (\sigma_{\mathrm{C}i,m,l} + \sigma_{\mathrm{C}i,r,l})$	root – mycorrhizal N,P transfer driven by $\sigma_{\mathrm{N,P}}$ conc’n gradients	[C53]

Definition of Variables in Section 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 r, mycorrhizae m				
		variables			
A	leaf, root or mycorrhizalsurface area	$m^2\ m^{-2}$	[C1,C6b,C6d,C8b, C21,C23,C32,C33,C47]		
β	shape parameter for stomatal effects on CO_2 diffusion and non-stomatal effects on carboxylation	MPa^{-1}	[C4 C27,C35,]	-5.0	Grant and Flanagan (2007)
$\boldsymbol{B}_{\mathbf{j}}$	parameter such that $f_{\mathrm{tj}\boldsymbol{i}}$ = 1.0 at T_{c} = 298.15 K		[C10c]	17.354	
$\boldsymbol{B}_{\mathbf{kc}}$	parameter such that $f_{\mathrm{tkc}i}$ = 1.0 at T_{c} = 298.15 K		[C10d]	22.187	
$\boldsymbol{B}_{\mathbf{ko}}$	parameter such that $f_{\mathrm{tko}i}$ = 1.0 at T_{c} = 298.15 K		[C10e]	8.067	
$\boldsymbol{B}_{\mathbf{o}}$	parameter such that $f_{\mathrm{to}\boldsymbol{i}}$ = 1.0 at T_{c} = 298.15 K		[C10b]	24.212	
$\boldsymbol{B}_{\mathbf{v}}$	parameter such that $f_{\mathrm{tv}\boldsymbol{i}}$ = 1.0 at T_{c} = 298.15 K		[C10a, C22]	26.229	
C_{b}	[CO_2] in canopy air	$\mu mol\ mol^{-1}$	[C2,C5 C25,C28]		
C_{c}	[CO_2] in canopy chloroplasts in equilibrium with $C_{\mathrm{i}i,j,k,l,m,n,o}$	μM	[C6a,C7b]		
$C_{\mathrm{c(b4)}}$	[CO_2] in C_4 bundle sheath	μM	[C38,C39,C42,C44,C45b]		
$C_{\mathrm{c(m4)}}$	[CO_2] in C_4 mesophyll in equilibrium with $C_{\mathrm{i}i,j,k,l,m,n,o}$	μM	[C29,C30b,C39]		
$\boldsymbol{C}_{\mathbf{i}}'$	[CO_2] in canopy leaves when ψ_{ci} = 0	$\mu mol\ mol^{-1}$	[C5]	0.70 x C_{b}	Larcher (2001)
C_{i}	[CO_2] in canopy leaves	$\mu mol\ mol^{-1}$	[C2]		
$C_{\mathrm{i(m4)}}'$	[CO_2] in C_4 mesophyll air when ψ_{ci} = 0	$\mu mol\ mol^{-1}$	[C28]	0.45 x C_{b}	

$C_{i(m4)}$	[CO_2] in C_4 mesophyll air	μmol mol^{-1}	[C25]		
$C_{i,j,z=l}$	C content of leaf ($z = l$)	g C m^{-2}	[C18]		
$D_{e\ NH_{4}l}$	effective dispersivity-diffusivity of NH_4^+ during root uptake	m^2 h^{-1}	[C23]		
$D_{e\ NO_{3}l}$	effective dispersivity-diffusivity of NO_3^- during root uptake	m^2 h^{-1}	[C23]		
$D_{e\ PO_{4}l}$	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]	$(\pi L_{s,z} / \Delta z)^{-1/2}$	Grant (1998)
$\boldsymbol{E}_{\mathbf{N,P}}$	energy cost of nutrient uptake	g C g N^{-1} or P^{-1}	[C13]	2.15	Veen (1981)
$f_{C(c3)}$	C_3 product inhibition of RuBP carboxylation activity in C_4 bundle sheath or C_3 mesophyll	–	[C47,C48,C49]		
$f_{C(m4)}$	C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	–	[C32,C33,C34]		
$\boldsymbol{F}_{\mathbf{chl}}$	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]		
$f_{\lambda N}$	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ N translocated out of leaf or root before litterfall	–	[C19a,c]		
$f_{\lambda P}$	fraction of $\boldsymbol{X}_{\mathbf{mx}}$ P translocated out of leaf or root before litterfall	–	[C19b,d]		

$\boldsymbol{F}_{\mathbf{rubisco}}$	fraction of leaf protein in rubisco	-	[C6b,d]	0.125	
f_{ta}	temperature effect on $R_{\mathrm{a}i,j}$ and U	–	[C14,C22,C23]		
f_{tb}	temperature effect on carboxylation	–	[C6b,C10a]		
f_{tj}	temperature effect on electron transport		[C8b,C10c]		
f_{tkc}	temperature effect on $\boldsymbol{K}_{\mathbf{c}_i}$		[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}	inhibition of root or mycorrhizal N exudation	–	[C19f,h]		
f_{xP}	inhibition of root or mycorrhizal P exudation	–	[C19g,i]		
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–	[C6a,C7a,C9]		Medrano et al. (2002)
$f_{\psi \boldsymbol{i}}$	non-stomatal water effect on carboxylation	–	[C32,C33,C35C47,C48]		
$g_{s\mathrm{C}}$	conductance for shoot-root C transfer	h^{-1}	[C50]	calculated from root depth, axis number	Grant (1998)
$\boldsymbol{g}_{\boldsymbol{s}\mathbf{N,P}}$	rate constant for shoot-root N,P transfer	h^{-1}	[C51]	0.1	Grant (1998)
$\boldsymbol{g}_{\boldsymbol{r}\mathbf{C}}$	rate constant for root-mycorrhizal C transfer	h^{-1}	[C52]	0.1	Grant (1998)
$\boldsymbol{g}_{\boldsymbol{r}\mathbf{N,P}}$	rate constant for root-mycorrhizal N,P transfer	h^{-1}	[C53]	0.1	Grant (1998)
$\boldsymbol{H}_{\mathbf{aj}}$	energy of activation for electron transport	J mol^{-1}	[C10c]	43×10^3	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	
$\boldsymbol{H}_{\mathbf{dl}}$	energy of low temperature deactivation	J mol^{-1}	[C10, C22]	197.5 x 10^3	
$[H_2PO_4{}^-{}_{i,r,l}]$	concentration of $H_2PO_4^-$ root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{H_2PO_4{}^-{}_{mn}}]$	concentration of $H_2PO_4^-$ at root or mycorrizal surfaces below which $U_{PO_4} = 0$	g N m^{-3}	[C23]	0.002	Barber and Silberbush, 1984
I	irradiance	µmol m^{-2} s^{-1}	[C8a,]		
J	electron transport rate in C$_3$ mesophyll	µmol m^{-2} s^{-1}	[C7a,C8a]		
$J_{(b4)}$	electron transport rate in C$_4$ bundle sheath	µmol m^{-2} s^{-1}	[C45a,C46]		
$J_{(m4)}$	electron transport rate in C$_4$ mesophyll	µmol m^{-2} s^{-1}	[C30a,C31]		
J_{max}'	specific electron transport rate at non-limiting I and 25^{o}C when $\psi_{ci} = 0$ and nutrients are nonlimiting	µmol g^{-1} s^{-1}	[C33,C48]	400	
$J_{max(b4)}$	electron transport rate in C$_4$ bundle sheath at non-limiting I	µmol m^{-2} s^{-1}	[C46,C48]		
$J_{max(m4)}$	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, ψ_{ci}, 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^{o}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^{o}C	Lawlor (1993)

$\boldsymbol{K}_{\mathbf{c}}$	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]		
$\boldsymbol{K}_{\mathbf{iC_N}}$	inhibition constant for growth in shoots from σ_{C} *vs.* σ_{N}	g C g N^{-1}	[C11]	100	Grant (1998)
$\boldsymbol{K}_{\mathbf{iC_P}}$	inhibition constant for growth in shoots from σ_{C} *vs.* σ_{P}	g C g P^{-1}	[C11]	1000	Grant (1998)
$K_{\mathrm{I}\chi\mathrm{C4(b4)}}$	constant for CO_2 product inhibition of C_4 decarboxylation in C_4 bundle sheath	μM	[C38]	1000.0	
$K_{\mathrm{I}\chi\mathrm{C4(m4)}}$	constant for C_4 product inhibition of PEP carboxylation activity in C_4 mesophyll	μM	[C34]	5 x 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 (1998)
$\boldsymbol{K}_{\mathbf{iP_C}}$	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 (1998)
$\boldsymbol{K}_{\boldsymbol{\lambda}\mathbf{N}}$	inhibition constant for remobilization of leaf or root N during senescence	g N g C^{-1}	[C19c]	0.1	
$\boldsymbol{K}_{\boldsymbol{\lambda}\mathbf{P}}$	inhibition constant for remobilization of leaf or root P during senescence	g P g C^{-1}	[C19d]	0.01	
$\boldsymbol{K}_{\mathbf{NH_4}}$	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]	0.32	Griffin (1972)

$\boldsymbol{K}_{\mathbf{o}}$	inhibition constant for O_2 in carboxylation	μM	[C6c,C6e]	500 at 25 °C	Farquhar et al. (1980)
$\boldsymbol{K}_{\mathbf{xN}}$	inhibition constant for exudation of root or mycorrhizal N	g C g N^{-1}	[C19h]	1.0	
$\boldsymbol{K}_{\mathbf{xP}}$	inhibition constant for exudation of root or mycorrhizal P	g C g N^{-1}	[C19i]	10.0	
L	root length	m m^{-2}	[C14d,C21b,C23]		
l_{C}	C litterfall from leaf or root	g C m^{-2} h^{-1}	[C18,C19a,b,C20]		
$l_{\mathrm{N,P}}$	N or P litterfall from leaf or root	g C m^{-2} h^{-1}	[C19a,b]		
M_{B}	branch C phytomass	g C m^{-2}	[C20,C50]		
M_{L}	leaf C phytomass	g C m^{-2}	[C12,C21]		
$M_{\mathrm{L_N}}$, $M_{\mathrm{L_R}}$	non-remobilizable, remobilizable (protein) leaf C phytomass	g C m^{-2}	[C12,C18]		
M_{M}	mycorrhizal C phytomass	g C m^{-2}	[C52]		
M_{R}	root C phytomass	g C m^{-2}	[C20,C21,C50,C52]		
$M_{\mathrm{L}_{iprot}}$	leaf protein phytomass calculated from leaf N, P contents	g N m^{-2}	[C6b,C6d,C8b]		
N,P	N or P content of organ *z*	g N m^{-2}	[C16, C19]		
$\boldsymbol{N}_{\mathbf{leaf}}$	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]		
$\mathbf{N}_{\mathbf{prot}}$	N content of protein remobilized from leaf or root	g N C^{-1}	[C12,C19a]	0.4	
$[N_{\mathrm{chl(b4)}}]'$	ratio of chlorophyll N in 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 C_4 mesophyll to total leaf N	g N g N^{-1}	[C33]	0.05	

$[NH_4^+{}_{i,r,l}]$	concentration of NH_4^+ at root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{NH_4^+{}_{mn}}]$	concentration of NH_4^+ at root or mycorrizal surfaces below which $U_{NH_4} = 0$	g N m^{-3}	[C23]	0.0125	Barber and Silberbush, 1984
$[NO_3^-{}_{i,r,l}]$	concentration of NH_4^+ at root or mycorrizal surfaces	g N m^{-3}	[C23]		
$[\mathbf{NO_3^-{}_{mn}}]$	concentration of NO_3^- at root or mycorrizal surfaces below which $U_{NO_3} = 0$	g N m^{-3}	[C23]	0.03	Barber and Silberbush, 1984
$[N_{pep(m4)}]'$	ratio of PEP carboxylase N in C_4 mesophyll to total leaf N	g N g N^{-1}	[C32]	0.025	
$[N_{rub(b4)}]'$	ratio of RuBP carboxylase N in C_4 bundle sheath to total leaf N	g N g N^{-1}	[C47]	0.025	
O_{2q}	aqueous O_2 concentration in root or mycorrhizal aerenchyma	g m^{-3}	[C14c,d]		
O_{2r}	aqueous O_2 concentration at root or mycorrhizal surfaces	g m^{-3}	[C14c,d]		
O_{2s}	aqueous O_2 concentration in soil solution	g m^{-3}	[C14c,d]		
O_c	$[O_2]$ in canopy chloroplasts in equilibrium with $O_{2\ in}$ atm.	μM	[C6c,C6e]		
$\boldsymbol{P}_{\mathbf{leaf}}$	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 $\boldsymbol{P}_{\mathbf{leaf}}$	
$\mathbf{P_{prot}}$	P content of protein remobilized from leaf or root	g P C^{-1}	[C12,C19b]	0.04	
$[\pi_{lf}]$	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_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]		
$\boldsymbol{R}_c'$	specific autotrophic respiration of $\sigma_{Ci,j}$ at T_{ci} = 25 °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]		
$\boldsymbol{R_{\mathrm{m}}'}$	specific maintenance respiration of $\sigma_{\mathrm{C}i,j}$ at $T_{\mathrm{c}i} = 25\ ^{\mathrm{o}}\mathrm{C}$	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,C23 a,c,e]	1.0×10^{-4} or 5.0×10^{-6}	
$R_{\mathrm{s}i,j}$	respiration from remobilization of leaf C	g C m^{-2} h^{-1}	[C13,C15,C18, C20]		
$r_{\mathrm{s}l}$	thickness of soil water films	m	[C14d]		
$\boldsymbol{r_x}$	rate constant for root or mycorrhizal exudation	h^{-1}	[C19f,g,h]	0.001	
ρ_r	dry matter content of root biomass	g g^{-1}	[C21b]	0.125	
$\boldsymbol{S}$	change in entropy	J mol^{-1} K^{-1}	[C10, C22]	710	Sharpe and DeMichelle (1977)
σ_{C}	nonstructural C product of CO_2 fixation	g C g C^{-1}	[C11,C19c,d,e,h,i, C23g,h,C50-53]		

σ_{N}	nonstructural N product of root uptake	g N g C^{-1}	[C11, C19c,f,h,i C23g,h,C51,C53]		
σ_{P}	nonstructural P product of root uptake	g P g C^{-1}	[C11, C19d,g,h,i C23g,h,C51,C53]		
T_{c}	canopy temperature	K	[C10, C22]		
$U_{\mathrm{NH4}i,r,l}$	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 °C and non-limiting NH_4^+	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush, 1984
$U_{\mathrm{NO3}i,r,l}$	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 °C and non-limiting NO_3^-	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush, 1984
$U_{\mathrm{PO4}i,r,l}$	$H_2PO_4^-$ uptake by roots or mycorrhizae	g N m^{-2} h^{-1}	[C23]		
$\boldsymbol{U'_{\mathrm{PO_4}}}$	maximum $U_{\mathrm{PO_4}}$ at 25 °C and non-limiting $H_2PO_4^-$	g N m^{-2} h^{-1}	[C23]	5.0 x 10^{-3}	Barber and Silberbush, 1984
$U_{\mathrm{O2}i,r,l}$	O_2 uptake by roots and mycorrhizae under ambient O_2	g O m^{-2} h^{-1}	[C14b,c,C23b,d,f]		
$U'_{\mathrm{O2}i,l.r}$	O_2 uptake by roots and mycorrhizae under nonlimiting O_2	g O m^{-2} h^{-1}	[C14b,c,C23b,d,f]		
$U_{\mathrm{w}i,r,l}$	root water uptake	m^{3} m^{-2} h^{-1}	[C14d,C23]		
$V_{\phi(\mathrm{b4})i,j,k}$	CO_2 leakage from C_4 bundle sheath to C_4 mesophyll	g C m^{-2} h^{-1}	[C39,C42]		
$\boldsymbol{V_{\mathrm{b}}'}$	specific rubisco carboxylation at 25 °C	µmol g^{-1} rubisco s^{-1}	[C6b]	45	Farquhar et al. (1980)
$V_{\mathrm{b(b4)}i,j,k}$	CO_2-limited carboxylation rate in C_4 bundle sheath	µmol m^{-2} s^{-1}	[C43,C44]		
$V_{\mathrm{b(m4)}i,j,k,l,m,n,o}$	CO_2-limited carboxylation rate in C_4 mesophyll	µmol m^{-2} s^{-1}	[C26]		
$V_{\mathrm{b}i,j,k,l,m,n,o}$	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 $\psi_{ci} = 0$ 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 $\psi_{ci} = 0$ 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, ψ_{ci}, 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]		
$V_{\mathrm{c_0(m4)}\ i,j,k,l,m,n,o}$	CO_2 fixation rate in C_4 mesophyll when $\psi_{ci} = 0$ 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 $\psi_{ci} = 0$	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]		
$\mathbf{V_j}'$	specific chlorophyll e^- transfer at 25 °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,C45a]		
$V_{\mathrm{j(m4)}i,j,k,l,m,n,o}$	irradiance-limited carboxylation rate in C_4 mesophyll	µmol m^{-2} s^{-1}	[C26,C30a]		
$V_{\mathrm{j}i,j,k,l,m,n,o}$	irradiance-limited leaf carboxylation rate	µmol m^{-2} s^{-1}	[C3,C7a]		
$\mathbf{V_o}'$	specific rubisco oxygenation at 25 °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, ψ_{ci}, 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]		
X_{mx}	maximum fraction of remobilizable N or P translocated out of leaf or root during senescence	-	[C19a,b]	0.6	Kimmins (2004)
$x_{i,r,l,\mathrm{C}}$	root and mycorrhizal C exudation	g C m^{-2} h^{-1}	[C19e]		
$x_{i,r,l,\mathrm{N}}$	root and mycorrhizal C exudation	g N m^{-2} h^{-1}	[C19f]		
$x_{i,r,l,\mathrm{P}}$	root and mycorrhizal C exudation	g P m^{-2} h^{-1}	[C19g]		
Y	carboxylation yield from electron transport in C_3 mesophyll	μmol CO_2 μmol e^{-1}	[C7a,b]		
$Y_{\mathrm{(b4)}}$	carboxylation yield from electron transport in C_4 bundle sheath	μmol CO_2 μmol e^{-1}	[C45a,b]		
$Y_{\mathrm{(m4)}}$	carboxylation yield from electron transport in C_4 mesophyll	μmol CO_2 μmol e^{-1}	[C30a,b]		
$\boldsymbol{Y}_{\mathbf{g}}$	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]		
$Z_{s\mathrm{C}}$	shoot-root C transfer	g C m^{-2} h^{-1}	[C50]		
$Z_{s\mathrm{N,P}}$	shoot-root N,P transfer	g N,P m^{-2} h^{-1}	[C51]		

$Z_{r\mathrm{C}}$	root-mycorrhizal C transfer	g C m^{-2} h^{-1}	[C52]		
$Z_{r\mathrm{N,P}}$	root-mycorrhizal N,P transfer	g N,P m^{-2} h^{-1}	[C53]		
$\mathit{\Gamma}$	CO_2 compensation point in C_3 mesophyll	μM	[C6a,C6c,C7b]		
$\mathit{\Gamma}_{\mathrm{(b4)}}$	CO_2 compensation point in C_4 bundle sheath	μM	[C44,C45b]		
$\mathit{\Gamma}_{\mathrm{(m4)}}$	CO_2 compensation point in C_4 mesophyll	μM	[C29,C30b]		
$\boldsymbol{\alpha}$	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)
$\chi_{\mathrm{C4(b4)}}$	non-structural C_4 fixation product in C_4 bundle sheath	g C m^{-2}	[C37,C38,C41]		
$\chi_{\mathrm{C4(m4)}}$	non-structural C_4 fixation product in C_4 mesophyll	g C m^{-2}	[C37,C40]		
$[\chi_{\mathrm{c3(b4)}}]$	concentration of non-structural C_3 fixation product in C_4 bundle sheath	g g^{-1}	[C49]		
$[\chi_{\mathrm{C4(m4)}}]$	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)
$\kappa_{\mathrm{Cc(b4)}}$	conductance to CO_2 leakage from C_4 bundle sheath	h^{-1}	[C39]	20	
ψ_{t}	canopy turgor potential	MPa	[C4]	1.25 at $\psi_{\mathrm{c}} = 0$	

Section 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) and *y* (NS) directions	[D1]
$Q_{\mathrm{r}y(x,y)} = v_{y(x,y)}\, d_{\mathrm{m}x,y}\, L_{x(x,y)}$		
$d_{x,y} = \max(0, d_{\mathrm{w}(x,y)} + d_{\mathrm{i}(x,y)} - d_{\mathrm{s}(x,y)})\, d_{\mathrm{w}(x,y)} / (d_{\mathrm{w}(x,y)} + d_{\mathrm{i}(x,y)})$	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	
$\Delta(d_{\mathrm{w}(x,y)} A_{x,y}) / \Delta t = Q_{\mathrm{r},x(x,y)} - Q_{\mathrm{r},x+1(x,y)} + Q_{\mathrm{r},y(x,y)} - Q_{\mathrm{r},y+1(x,y)} + \mathrm{P} - \mathrm{E}_{x,y} - Q_{\mathrm{w}z(x,y,1)}$	2D kinematic wave theory for overland flow	[D4]
$R = s_\mathrm{r}\, d_\mathrm{m} / [2\,(s_\mathrm{r}^2 + 1)\; 0.5]$	wetted perimeter	[D5a]
$s_{x(x,y)} = 2\, abs[(Z + d_\mathrm{s} + d_\mathrm{m})_{x,y} - (Z + d_\mathrm{s} + d_\mathrm{m})_{x+1,y}] / (L_{x(x,y)} + L_{x(x+1,y)})$	2D slope from topography and pooled surface water in *x* (EW) and *y* (NS) directions	[D5b]
$s_{y(x,y)} = 2\, abs[(Z + d_\mathrm{s} + d_\mathrm{m})_{x,y} - (Z + d_\mathrm{s} + d_\mathrm{m})_{x,y+1}] / (L_{y(x,y)} + L_{y(x,y+1)})$		
$\boldsymbol{L}E_\mathrm{l} = L\,(e_\mathrm{a} - e_{\mathrm{l}(T_l,\psi_l)}) / r_{\mathrm{a}l}$	evaporation from surface litter	[D6a]
$\boldsymbol{L}E_\mathrm{s} = L\,(e_\mathrm{a} - e_{\mathrm{s}(T_s,\psi_s)}) / r_{\mathrm{as}}$	evaporation from soil surface	[D6b]

Subsurface Water Flux

$Q_{\mathrm{w}x(x,y,z)} = K'_x\,(\psi_{sx,y,z} - \psi_{sx+1,y,z})$	3D Richard's or Green-Ampt equation depending on saturation of source or target cell in *x* (EW),	[D7]
$Q_{\mathrm{w}y(x,y,z)} = K'_y\,(\psi_{sx,y,z} - \psi_{sx,y+1,z})$		

$Q_{wz(x,y,z)} = K'_z\,(\psi_{sx,y,z} - \psi_{sx,y,z+1})$	*y* (NS) and *z* (vertical) directions	
$\Delta\theta_{w\,x,y,z}/\Delta t = (Q_{wx(x,y)} - Q_{wx+1(x,y)} + Q_{wy(x,y)} - Q_{wy+1(x,y)} + Q_{wz(x,y)} - Q_{wz+1(x,y)} + Q_{f(x,y,z)}) / L_{z(x,y,z)}$	3D water transfer plus freeze-thaw	[D8]
$K'_x = 2\,K_{x,y,z}\,K_{x+1,y,z} / (K_{x,y,z}\,L_{x,(x+1,y,z)} + K_{x+1,y,z}\,L_{x,(x,y,z)})$	in direction *x* if source and destination cells are unsaturated	[D9a]
$= 2\,K_{x,y,z} / (L_{x(x+1,y,z)} + L_{x(x,y,z)})$	in direction *x* if source cell is saturated	[D9b]
$= 2\,K_{x+1,y,z} / (L_{x(x+1,y,z)} + L_{x(x,y,z)})$	in direction *x* if destination cell is saturated	
$K'_y = 2\,K_{x,y,z}\,K_{x,y+1,z} / (K_{x,y,z}\,L_{y(x,y+1,z)} + K_{x,y+1,z}\,L_{y(x,y,z)})$	in direction *y* if source and destination cells are unsaturated	[D9a]
$= 2\,K_{x,y,z} / (L_{y(x,y+1,z)} + L_{y(x,y,z)})$	in direction *y* if source cell is saturated	[D9b]
$= 2\,K_{x,y+1,z} / (L_{y(x,y+1,z)} + L_{y(x,y,z)})$	in direction *y* if destination cell is saturated	
$K'_z = 2\,K_{x,y,z}\,K_{x,y,z+1} / (K_{x,y,z}\,L_{z(x,y,z+1)} + K_{x,y,z+1}\,L_{z(x,y,z)})$	in direction *z* if source and destination cells are unsaturated	[D9a]
$= 2\,K_{x,y,z} / (L_{z(x,y,z+1)} + L_{z(x,y,z)})$	in direction *z* if source cell is saturated	[D9b]
$= 2\,K_{x,y,z+1} / (L_{z(x,y,z+1)} + L_{z(x,y,z)})$	in direction *z* if destination cell is saturated	

Exchange with Water Table

$Q_{tx(x,y,z)} = K_{x,y,z}\,[\psi' - \psi_{sx,y,z} + 0.01\,(d_{zx,y,z} - d_t)] / (L_{tx} + 0.5\,L_{x,(x,y,z)})$	if $\psi_{sx,y,z} > \psi' + 0.01(d_{zx,y,z} - d_t)$ for all depths *z* from $d_{zx,y,z}$ to d_t	[D10]
$Q_{ty(x,y,z)} = K_{x,y,z}\,[\psi' - \psi_{sx,y,z} + 0.01\,(d_{zx,y,z} - d_t)] / (L_{ty} + 0.5\,L_{y,(x,y,z)})$	or if $d_{zx,y,z} > d_t$	

Heat Flux

$R_n + \boldsymbol{L}E + H + G = 0$	for eachcanopy, snow, residue and soil surface, depending on exposure	[D11]
$G_{x(x,y,z)} = 2\,\kappa_{(x,y,z),(x+1,y,z)}\,(T_{(x,y,z)} - T_{(x+1,y,z)}) / (L_{x\,(x,y,z)} + L_{x\,(x+1,y,z)}) + c_w\,T_{(x,y,z)}\,Q_{wx(x,y,z)}$	3D conductive – convective heat flux among snowpack, surface	[D12a]
$G_{y(x,y,z)} = 2\,\kappa_{(x,y,z),(x,y+1,z)}\,(T_{(x,y,z)} - T_{(x,y+1,z)}) / (L_{y\,(x,y,z)} + L_{y\,(x,y+1,z)}) + c_w\,T_{(x,y,z)}\,Q_{wy(x,y,z)}$	residue and soil layers in *x* (EW), *y*	[D12b]

$G_{z(x,y,z)} = 2\ \kappa_{(x,y,z),(x,y,z+1)} (T_{(x,y,z)} - T_{(x,y,z+1)}) / (L_{z\,(x,y,z)} + L_{z\,(x,y,z+1)}) + c_w\, T_{(x,y,z)}\, Q_{\mathrm{wz}(x,y,z)}$	(NS) and *z* (vertical) directions	[D12c]
$G_{x(x-1,y,z)} - G_{x(x,y,z)} + G_{y(x,y-1,z)} - G_{y(x,y,z)} + G_{z(x,y,z-1)} - G_{z(x,y,z)} + \boldsymbol{L}Q_{f(x,y,z)} + c_{(x,y,z)} (T_{(x,y,z)} - T'_{(x,y,z)}) / \Delta t = 0$	3D general heat flux equation driving freezing-thawing in snowpack, surface residue and soil layers	[D13]

Gas Flux

$Q_{\mathrm{ds}\gamma x,y,z} = a_{\mathrm{gs}x,y,z}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, ft_{\mathrm{d}_{\gamma}x,y,z}\, [\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{ss}}]_{x,y,z})$	volatilization – dissolution between aqueous and gaseous phases in soil and root	[D14a]
$Q_{\mathrm{dr}\gamma x,y,z} = a_{\mathrm{gr}x,y,z}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, ft_{\mathrm{d}_{\gamma}x,y,z}\, [\gamma_{\mathrm{gr}}]_{x,y,z} - [\gamma_{\mathrm{sr}}]_{x,y,z})$		[D14b]
$Q_{\mathrm{gs}\gamma\mathrm{z}x,y,1} = g_{\mathrm{a}x,y}\, \{[\gamma_{\mathrm{a}}] - \{2\, [\gamma_{\mathrm{gs}}]_{x,y,1} D_{\mathrm{gs}\gamma z(x,y,1)} / L_{\mathrm{z}(x,y,1)} + g_{\mathrm{a}x,y}\, [\gamma_{\mathrm{a}}]\}/\{2\, D_{\mathrm{gs}\gamma\mathrm{z}(x,y,1)} / L_{\mathrm{z}(x,y,1)} + g_{\mathrm{a}x,y}\}\}$	volatilization – dissolution between gaseous and aqueous phases at the soil surface (*z = 1*) and the atmosphere	[D15a]
$Q_{\mathrm{ds}\gamma x,y,1} = a_{\mathrm{gs}x,y,1}\, D_{\mathrm{d}\gamma}\, (\boldsymbol{S}'_{\gamma}\, ft_{\mathrm{d}_{\gamma}x,y,1}\, [\gamma_{\mathrm{a}}] - [\gamma_{\mathrm{ss}}]_{x,y,1})$		[D15b]
$Q_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)} = - Q_{\mathrm{wx}(x,y,z)}\, [\gamma_{\mathrm{gs}}]_{x,y,z} + 2\, D_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)}\, ([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x+1,y,z}) / (L_{x\,(x,y,z)} + L_{x\,(x+1,y,z)})$	3D convective - conductive gas flux among soil layers in *x* (EW), *y* (NS) and *z* (vertical) directions,	[D16a]
$Q_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)} = - Q_{\mathrm{wy}(x,y,z)}\, [\gamma_{\mathrm{gs}}]_{x,y,z} + 2\, D_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)}\, ([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x,y+1,z}) / (L_{y\,(x,y,z)} + L_{y\,(x,y+1,z)})$		[D16b]
$Q_{\mathrm{gs}\gamma\mathrm{z}(x,y,z)} = - Q_{\mathrm{wz}(x,y,z)}\, [\gamma_{\mathrm{gs}}]_{x,y,z} + 2\, D_{\mathrm{g}\gamma\mathrm{z}(x,y,z)}\, ([\gamma_{\mathrm{gs}}]_{x,y,z} - [\gamma_{\mathrm{gs}}]_{x,y,z+1}) / (L_{z\,(x,y,z)} + L_{z\,(x,y,z+1)})$		[D16c]
$Q_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)} = D_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)}\, ([\gamma_{\mathrm{gr}}]_{x,y,z} - [\gamma_{\mathrm{a}}])/ \Sigma_{1,\mathrm{z}}\, L_{z\,(x,y,z)}$	convective - conductive gas flux between roots and the atmosphere	[D16d]
$D_{\mathrm{gs}\gamma\mathrm{x}(x,y,z)} = \boldsymbol{D}'_{\mathbf{g}\gamma}\ ft_{\mathrm{g}x,y,z}\, [0.5\, (\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x+1,y,z})]^2 / \theta_{\mathrm{ps}x,y,z}{}^{0.67}$	gasous diffusivity as a function of air-filled porosity in soil	[D17a]
$D_{\mathrm{gs}\gamma\mathrm{y}(x,y,z)} = \boldsymbol{D}'_{\mathbf{g}\gamma}\ ft_{\mathrm{g}x,y,z}\, [0.5\, (\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x,y+1,z})]^2 / \theta_{\mathrm{ps}x,y,z}{}^{0.67}$		[D17b]
$D_{\mathrm{gs}\gamma\mathrm{z}(x,y,z)} = \boldsymbol{D}'_{\mathbf{g}\gamma}\ ft_{\mathrm{g}x,y,z}\, [0.5\, (\theta_{\mathrm{g}x,y,z} + \theta_{\mathrm{g}x,y,z+1})]^2 / \theta_{\mathrm{ps}x,y,z}{}^{0.67}$		[D17c]
$D_{\mathrm{gr}\gamma\mathrm{z}(x,y,z)} = \boldsymbol{D}'_{\mathbf{g}\gamma}\ ft_{\mathrm{g}x,y,z}\, \boldsymbol{\theta}_{\mathbf{pr}x,y,z}{}^{1.33}\, \mathrm{A}_{\mathrm{r}\,(x,y,z)} / \mathrm{A}_{x,y}$	gasous diffusivity as a function of air-filled porosity in roots	[D17d]

$Q_{\mathrm{b}\gamma\mathrm{z}} = \min[0.0,\ \{(44.64\ \theta_{wx,y,z}\ 273.16 / T_{(x,y,z)}) - \Sigma_\gamma ([\gamma_\mathrm{s}]_{x,y,z} / (\boldsymbol{S}'_\gamma\ ft_{\mathrm{d}_\gamma x,y,z} M_\gamma))\}]$ $([\gamma_\mathrm{s}]_{x,y,z} / (\boldsymbol{S}'_\gamma\ ft_{\mathrm{d}_\gamma x,y,z} M_\gamma)) / \Sigma_\gamma ([\gamma_\mathrm{s}]_{x,y,z} / (\boldsymbol{S}'_\gamma\ ft_{\mathrm{d}_\gamma x,y,z} M_\gamma))\ \boldsymbol{S}'_\gamma\ ft_{\mathrm{d}_\gamma x,y,z} M_\gamma\ V_{x,y,z}$	bubbling (-ve flux) when total of all partial gas pressures exceeds atmospheric pressure	[D18]

Solute Flux

$Q_{\mathrm{s}\gamma\mathrm{x}(x,y,z)} = -\ Q_{\mathrm{wx}(x,y,z)}\ [\gamma_\mathrm{ss}]_{x,y,z} + 2\ D_{\mathrm{s}\gamma\mathrm{x}(x,y,z)}\ ([\gamma_\mathrm{s}]_{x,y,z} - [\gamma_\mathrm{s}]_{x+1,y,z}) / (L_{x\ (x,y,z)} + L_{x\ (x+1,y,z)})$	3D convective - dispersive solute flux among soil layers in *x* (EW), *y* (NS) and *z* (vertical) directions	[D19a]
$Q_{\mathrm{s}\gamma\mathrm{y}(x,y,z)} = -\ Q_{\mathrm{wy}(x,y,z)}\ [\gamma_\mathrm{ss}]_{x,y,z} + 2\ D_{\mathrm{s}\gamma\mathrm{y}(x,y,z)}\ ([\gamma_\mathrm{s}]_{x,y,z} - [\gamma_\mathrm{s}]_{x,y+1,z}) / (L_{y\ (x,y,z)} + L_{y\ (x,y+1,z)})$		[D19b]
$Q_{\mathrm{s}\gamma\mathrm{z}(x,y,z)} = -\ Q_{\mathrm{wz}(x,y,z)}\ [\gamma_\mathrm{ss}]_{x,y,z} + 2\ D_{\mathrm{s}\gamma\mathrm{z}(x,y,z)}\ ([\gamma_\mathrm{s}]_{x,y,z} - [\gamma_\mathrm{s}]_{x,y,z+1}) / (L_{z\ (x,y,z)} + L_{z\ (x,y,z+1)})$		[D19c]
$Q_{\mathrm{r}\gamma(x,y,z)} = -\ Q_{\mathrm{wr}(x,y,z)}\ [\gamma_\mathrm{ss}]_{x,y,z} + 2\pi\ L_{i,r}\ D_{\mathrm{s}\gamma}([\gamma_\mathrm{ss}] - [\gamma_{\mathrm{rr}i,r}])\ \ln\{(r_\mathrm{s} + r_{\mathrm{r}i,r}) / r_{\mathrm{r}i,r}\}$ $+ 2\pi\ L_{i,r}\ D_{\mathrm{r}\gamma}([\gamma_{\mathrm{sr}i,r}] - [\gamma_{\mathrm{rr}i,r}])\ \ln(r_{\mathrm{q}i,r}) / r_{\mathrm{r}i,r})$	convective - dispersive solute flux between soil and root aqueous phases	[D19d]
$D_{\mathrm{s}\gamma\mathrm{x}(x,y,z)} = D_{\mathrm{qx}(x,y,z)}\ \lvert Q_{\mathrm{wx}(x,y,z)} \rvert + \boldsymbol{D'}_{\mathbf{s}\gamma}\ ft_{\mathrm{s}x,y,z}\ [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$	aqueous dispersivity in soil as functions of water flux and water-filled porosity in *x*, *y* and *z* directions	[D20a]
$D_{\mathrm{s}\gamma\mathrm{y}(x,y,z)} = D_{\mathrm{qy}(x,y,z)}\ \lvert Q_{\mathrm{wy}(x,y,z)} \rvert + \boldsymbol{D'}_{\mathbf{s}\gamma}\ ft_{\mathrm{s}x,y,z}\ [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$		[D20b]
$D_{\mathrm{s}\gamma\mathrm{z}(x,y,z)} = D_{\mathrm{qz}(x,y,z)}\ \lvert Q_{\mathrm{wz}(x,y,z)} \rvert + \boldsymbol{D'}_{\mathbf{s}\gamma}\ ft_{\mathrm{s}x,y,z}\ [0.5(\theta_{\mathrm{w}x,y,z} + \theta_{\mathrm{w}x+1,y,z})]\ \tau$		[D20c]
$D_{\mathrm{r}\gamma(x,y,z)} = \boldsymbol{D'}_{\mathbf{qr}}\ \lvert Q_{\mathrm{wr}(x,y,z)} \rvert + \boldsymbol{D'}_{\mathbf{s}\gamma}\ ft_{\mathrm{s}x,y,z}\ \theta_{\mathrm{w}x,y,z}\ \tau$	aqueous dispersivity to roots as functions of water flux and water-filled porosity	[D20d]
$D_{\mathrm{qx}(x,y,z)} = 0.5\ \boldsymbol{\alpha}\,(L_{x\ (x,y,z)} + L_{x\ (x+1,y,z)})^{\boldsymbol{\beta}}$	dispersivity as a function of water flow length	[D21a]
$D_{\mathrm{qy}(x,y,z)} = 0.5\ \boldsymbol{\alpha}\,(L_{y\ (x,y,z)} + L_{y\ (x,y+1,z)})^{\boldsymbol{\beta}}$		[D21b]
$D_{\mathrm{qz}(x,y,z)} = 0.5\ \boldsymbol{\alpha}\,(L_{z\ (x,y,z)} + L_{z\ (x,y,z+1)})^{\boldsymbol{\beta}}$		[D21c]

Definition of Variables in Section 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	m^2	[D17c]		
A_r	root cross-sectional area of landscape position	m^2	[D17c]		
a_{gr}	air-water interfacial area in roots	$m^2\ m^{-2}$	[D14b]		
a_{gs}	air-water interfacial area in soil	$m^2\ m^{-2}$	[D14a,D15b]		Skopp (1985)
$\boldsymbol{\alpha}$	dependence of D_q on L	-	[D21]	0.20	
$\boldsymbol{\beta}$	dependence of D_q on L	-	[D21]	1.07	
c	heat capacity of soil	MJ $m^{-2}\ {}^oC^{-1}$	[D13]		
c_w	heat capacity of water	MJ $m^{-3}\ {}^oC^{-1}$	[D12]	4.19	
$D_{d\gamma}$	volatilization - dissolution transfer coefficient for gas γ	$m^2\ h^{-1}$	[D14,D15a]		
$D_{gr\gamma}$	gaseous diffusivity of gas γ in roots	$m^2\ h^{-1}$	[D16d,D17d]		Luxmoore et al. (1970a,b)
$D_{gs\gamma}$	gaseous diffusivity of gas γ in soil	$m^2\ h^{-1}$	[D15a,D16a,b,c,D17a,b,c]		Millington and Quirk (1960)
$\mathbf{D'}_{g\gamma}$	diffusivity of gas γ in air at 0 ^oC	$m^2\ h^{-1}$	[D17]	6.43×10^{-2} for $\gamma = O_2$	Campbell (1985)

$\boldsymbol{D'}_{\mathbf{qr}}$	dispersivity in roots	m	[D20d]	0.004	
D_{q}	dispersivity in soil	m	[D20,D21]		
$D_{\mathrm{r}\gamma}$	aqueous diffusivity of gas or solute γ in roots	$\mathrm{m^2\ h^{-1}}$	[D19d,D20d]		
$D_{\mathrm{s}\gamma}$	aqueous diffusivity of gas or solute γ in soil	$\mathrm{m^2\ h^{-1}}$	[D19,D20]		
$\boldsymbol{D'}_{\mathbf{s}\gamma}$	diffusivity of gas γ in water at 0 $^{\mathrm{o}}$C	$\mathrm{m^2\ h^{-1}}$	[D20]	8.57×10^{-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]		
d_{t}	depth of external water table	m	[D10]		
d_{w}	depth of surface water	m	[D1,D2]		
d_{z}	depth to mid-point of soil layer	m	[D10]		
E	evaporation or transpiration flux	$\mathrm{m^3\ m^{-2}\ h^{-1}}$	[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}	$\mathrm{g\ m^{-3}}$	[D6a]		
$e_{\mathrm{s}(T_s,\psi_s)}$	soil surface vapor density at current T_{s} and ψ_{s}	$\mathrm{g\ m^{-3}}$	[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	$\mathrm{m^3\ m^{-2}\ h^{-1}}$	[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 Section E)		[D14,D15]	
$[\gamma_a]$	atmospheric concentration of gas γ	g m^{-3}	[D15,D16d]	
$[\gamma_{gr}]$	gasous concentration of gas γ in roots	g m^{-3}	[D14b,D16d]	
$[\gamma_{gs}]$	gasous concentration of gas γ in soil	g m^{-3}	[D14a,D15a,D16a,D16b,D16c]	
$[\gamma_{sr}]$	aqueous concentration of gas γ in roots	g m^{-3}	[D14b, D19d]	
$[\gamma_{rr}]$	aqueous concentration of gas γ at root surface	g m-3	[D19b]	
$[\gamma_{ss}]$	aqueous concentration of gas γ in soil	g m^{-3}	[D14a,D15b,D18, D19]	
H	sensible heat flux	MJ m^{-2} h^{-1}	[D11]	
K	hydraulic conductivity	m^2 MPa^{-1} h^{-1}	[D9,D10]	Green and Corey (1971)
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_i	root length	m m^{-2}	[D19d]	
L_t	distance from boundary to external water table in *x* or *y* directions	m	[D10]	
L_x , L_y , L_z	length of landscape element in *x*, *y* or *z* directions	m	[D1,D5b,D8,D9,D10,D12,D15a,D16,D19]	
$\boldsymbol{L}E_l$	latent heat flux from surface litter	[D6a]	MJ m^{-2} h^{-1}	
$\boldsymbol{L}E_s$	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]		
$Q_{\mathrm{b}\gamma z}$	bubbling flux	g m^{-2} h^{-1}	[D18]		
$Q_{\mathrm{dr}\gamma}$	volatilization – dissolution of gas γ between aqueous and gaseous phases in roots	g m^{-2} h^{-1}	[D14b]		
$Q_{\mathrm{ds}\gamma}$	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]		
$Q_{\mathrm{gr}\gamma}$	gaseous flux of gas γ between roots and the atmosphere	g m^{-2} h^{-1}	[D16d]		
$Q_{\mathrm{gs}\gamma}$	gaseous flux of gas γ in soil	g m^{-2} h^{-1}	[D15a,D16a,b,c]		
$Q_{\mathrm{r}x}$, $Q_{\mathrm{r}y}$	surface water flow in x or y directions	m^{3} m^{-2} h^{-1}	[D1,D4]		
$Q_{\mathrm{s}\gamma}$	aqueous flux of gas or solute γ in soil	g m^{-2} h^{-1}	[D19a,b,c]		
$Q_{\mathrm{r}\gamma}$	aqueous flux of gas or solute γ from soil and root aqueous phases to root surface	g m^{-2} h^{-1}	[D19d]		
Q_{t}	water flux between boundary grid cell and external water table in x or y directions	m^{3} m^{-2} h^{-1}	[D10]		
$Q_{\mathrm{w}r}$	root water uptake	m^{3} m^{-2} h^{-1}	[D19d, D20d]		
$Q_{\mathrm{w}x}$,$Q_{\mathrm{w}y}$,Q_{wz}	subsurface water flow in x, y or z directions	m^{3} m^{-2} h^{-1}	[D4,D7,D8,D12,D16,D19,D20]		
θ_{g}	air-filled porosity	m^{3} m^{-3}	[D17a,b,c]		
$\boldsymbol{\theta}_{\mathbf{pr}}$	root porosity	m^{3} m^{-3}	[D17d]	dryland spp. 0.10 wetland spp. 0.20	Luxmoore et al. (1970a,b)
θ_{ps}	soil porosity	m^{3} m^{-3}	[D17a,b,c]		
θ_{w}	water-filled porosity	m^{3} m^{-3}	[D8,D18,D20]		

R	ratio of cross-sectional area to perimeter of surface flow	m	[D3,D5a]		
R_n	net radiation	MJ m^{-2} h^{-1}	[D11]		
r_{al}	surface litter boundary layer resistance	m h^{-1}	[D6a]		
r_{as}	Soil surface boundary layer resistance	m h^{-1}	[D6b]		
$r_{\mathrm{q}i,r}$	radius of root or mycorrhizal aerenchyma	m	[D19d]		
$r_{\mathrm{r}i,r}$	root or mycorrhizal radius	m	[D19d]	1.0×10^{-4} or 5.0×10^{-6}	
r_{s}	thickness of soil water films	m	[D19d, D21d]		
$\boldsymbol{S}'_{\gamma}$	Ostwald solubility coefficient of gas γ at 30 $^{\mathrm{o}}$C	-	[D14,D15b,D18]	0.0293 for $\gamma = O_2$	Wilhelm et al. (1977)
s_{r}	slope of channel sides during surface flow	m m^{-1}	[D5a]		
s_x , s_y	slope in x or y directions	m m^{-1}	[D3,D5b]		
T	soil temperature	$^{\mathrm{o}}$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]	5.0×10^{-3}	
ψ_{s}	soil water potential	MPa	[D7,D10]		
Z	surface elevation	m	[D5b]		
z_{r}	Manning's roughness coefficient	$m^{-1/3}$ h	[D3]	0.01	

Section E: Solute Transformations

Precipitation - Dissolution Equilibria

$Al(OH)_{3(s)} \Leftrightarrow (Al^{3+}) + 3\,(OH^{-})$	(amorphous $Al(OH)_3$)	*-33.0*	[E1] [1]
$Fe(OH)_{3(s)} \Leftrightarrow (Fe^{3+}) + 3\,(OH^{-})$	(soil Fe)	*-39.3*	[E2]
$CaCO_{3(s)} \Leftrightarrow (Ca^{2+}) + (CO_3^{2-})$	(calcite)	-9.28	[E3]
$CaSO_{4(s)} \Leftrightarrow (Ca^{2+}) + (SO_4^{2-})$	(gypsum)	*-4.64*	[E4]
$AlPO_{4(s)} \Leftrightarrow (Al^{3+}) + (PO_4^{3-})$	(variscite)	*-22.1*	[E5] [2]
$FePO_{4(s)} \Leftrightarrow (Fe^{3+}) + (PO_4^{3-})$	(strengite)	*-26.4*	[E6]
$Ca(H_2PO_4)_{2(s)} \Leftrightarrow (Ca^{2+}) + 2\,(H_2PO_4^{-})$	(monocalcium phosphate)	*-1.15*	[E7] [3]
$CaHPO_{4(s)} \Leftrightarrow (Ca^{2+}) + (HPO_4^{2-})$	(monetite)	*-6.92*	[E8]
$Ca_5(PO_4)_3OH_{(s)} \Leftrightarrow 5\,(Ca^{2+}) + 3\,(PO_4^{3-}) + (OH^{-})$	(hydroxyapatite)	*-58.2*	[E9]

Cation Exchange Equilibria [4]

$X\text{-}Ca + 2\,(NH_4^{+}) \Leftrightarrow 2\,X\text{-}NH_4 + (Ca^{2+})$	*1.00*	[E10]
$3\,X\text{-}Ca + 2\,(Al^{3+}) \Leftrightarrow 2\,X\text{-}Al + 3\,(Ca^{2+})$	*1.00*	[E11]
$X\text{-}Ca + (Mg^{2+}) \Leftrightarrow X\text{-}Mg + (Ca^{2+})$	*0.60*	[E12]
$X\text{-}Ca + 2\,(Na^{+}) \Leftrightarrow 2\,X\text{-}Na + (Ca^{2+})$	*0.16*	[E13]
$X\text{-}Ca + 2\,(K^{+}) \Leftrightarrow 2\,X\text{-}K + (Ca^{2+})$	*3.00*	[E14]
$X\text{-}Ca + 2\,(H^{+}) \Leftrightarrow 2\,X\text{-}H + (Ca^{2+})$	*1.00*	[E15]

---

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

[2] All 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.

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

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

$3\ X\text{-}Al + 2\ (X\text{-}Ca + X\text{-}Mg) + X\text{-}NH_4 + X\text{-}K + X\text{-}Na + X\text{-}H = CEC$ [E16]

Anion Adsorption Equilibria

$X\text{-}OH_2^{+} \Leftrightarrow X\text{-}OH + (H^{+})$ *-7.35* [E17]

$X\text{-}OH \Leftrightarrow X\text{-}O^{-} + (H^{+})$ *-8.95* [E18]

$X\text{-}H_2PO_4 + H_2O \Leftrightarrow X\text{-}OH_2^{+} + (H_2PO_4^{-})$ *-2.80* [E19]

$X\text{-}H_2PO_4 + (OH^{-}) \Leftrightarrow X\text{-}OH + (H_2PO_4^{-})$ *4.20* [E20]

$X\text{-}HPO_4^{-} + (OH^{-}) \Leftrightarrow X\text{-}OH + (HPO_4^{2-})$ *2.60* [E21]

$X\text{-}OH_2^{+} + X\text{-}OH + X\text{-}O^{-} + X\text{-}H_2PO_4 + X\text{-}HPO_4^{-} + X\text{–}COO^{-} = AEC$ [E22]

Organic Acid Equilibria

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

Ion Pair Equilibria

$(NH_4^{+}) \Leftrightarrow (NH_3)_{(g)} + (H^{+})$ *-9.24* [E24]

$H_2O \Leftrightarrow (H^{+}) + (OH^{-})$ *-14.3* [E25]

$(CO_2)_{(g)} + H_2O \Leftrightarrow (H^{+}) + (HCO_3^{-})$ *-6.42* [E26]

$(HCO_3^{-}) \Leftrightarrow (H^{+}) + (CO_3^{2-})$ *-10.4* [E27]

$(AlOH^{2+}) \Leftrightarrow (Al^{3+}) + (OH^{-})$ *-9.06* [E28]

$(Al(OH)_2^{+}) \Leftrightarrow (AlOH^{2+}) + (OH^{-})$ *-10.7* [E29]

$(Al(OH)_3^{0}) \Leftrightarrow (Al(OH)_2^{+}) + (OH^{-})$ *-5.70* [E30]

$(Al(OH)_4^{-}) \Leftrightarrow (Al(OH)_3^{0}) + (OH^{-})$ *-5.10* [E31]

$(AlSO_4^{+}) \Leftrightarrow (Al^{3+}) + (SO_4^{2-})$ *-3.80* [E32]

$(FeOH^{2+}) \Leftrightarrow (Fe^{3+}) + (OH^{-})$ *-12.1* [E33]

$(Fe(OH)_2^{+}) \Leftrightarrow (FeOH^{2+}) + (OH^{-})$ *-10.8* [E34]

$(Fe(OH)_3^{0}) \Leftrightarrow (Fe(OH)_2^{+}) + (OH^{-})$ *-6.94* [E35]

$(Fe(OH)_4^{-}) \Leftrightarrow (Fe(OH)_3^{0}) + (OH^{-})$ *-5.84* [E36]

$(FeSO_4^{+}) \Leftrightarrow (Fe^{3+}) + (SO_4^{2-})$	*-4.15*	[E37]
$(CaOH^{+}) \Leftrightarrow (Ca^{2+}) + (OH^{-})$	*-1.90*	[E38]
$(CaCO_3^{0}) \Leftrightarrow (Ca^{2+}) + (CO_3^{2-})$	*-4.38*	[E39]
$(CaHCO_3^{+}) \Leftrightarrow (Ca^{2+}) + (HCO_3^{-})$	*-1.87*	[E40]
$(CaSO_4^{0}) \Leftrightarrow (Ca^{2+}) + (SO_4^{2-})$	*-2.92*	[E41]
$(MgOH^{+}) \Leftrightarrow (Mg^{2+}) + (OH^{-})$	*-3.15*	[E42]
$(MgCO_3^{0}) \Leftrightarrow (Mg^{2+}) + (CO_3^{2-})$	*-3.52*	[E43]
$(MgHCO_3^{+}) \Leftrightarrow (Mg^{2+}) + (HCO_3^{-})$	*-1.17*	[E44]
$(MgSO_4^{0}) \Leftrightarrow (Mg^{2+}) + (SO_4^{2-})$	*-2.68*	[E45]
$(NaCO_3^{-}) \Leftrightarrow (Na^{+}) + (CO_3^{2-})$	*-3.35*	[E46]
$(NaSO_4^{-}) \Leftrightarrow (Na^{+}) + (SO_4^{2-})$	*-0.48*	[E47]
$(KSO_4^{-}) \Leftrightarrow (K^{+}) + (SO_4^{2-})$	*-1.30*	[E48]
$(H_3PO_4) \Leftrightarrow (H^{+}) + (H_2PO_4^{-})$	*-2.15*	[E49]
$(H_2PO_4^{-}) \Leftrightarrow (H^{+}) + (HPO_4^{2-})$	*-7.20*	[E50]
$(HPO_4^{2-}) \Leftrightarrow (H^{+}) + (PO_4^{3-})$	*-12.4*	[E51]
$(FeH_2PO_4^{2+}) \Leftrightarrow (Fe^{3+}) + (H_2PO_4^{-})$	*-5.43*	[E52]
$(FeHPO_4^{+}) \Leftrightarrow (Fe^{3+}) + (HPO_4^{2-})$	*-10.9*	[E53]
$(CaH_2PO_4^{+}) \Leftrightarrow (Ca^{2+}) + (H_2PO_4^{-})$	*-1.40*	[E54]
$(CaHPO_4^{0}) \Leftrightarrow (Ca^{2+}) + (HPO_4^{2-})$	*-2.74*	[E55]
$(CaPO_4^{-}) \Leftrightarrow (Ca^{2+}) + (PO_4^{3-})$	*-6.46*	[E56]
$(MgHPO_4^{0}) \Leftrightarrow (Mg^{2+}) + (HPO_4^{2-})$	*-2.91*	[E57]

Section H: Inorganic N Transformations

Mineralization and Immobilization of Ammonium by All Microbial Populations

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

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

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

Oxidation of DOC and Reduction of Oxygen by Heterotrophs

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

$$R'_{\mathrm{O_2}i,h} = \mathbf{RQ_C}\,X'_{\mathrm{DOC}i,h} \qquad \text{[H3]}$$

$$R_{\mathrm{O_2}i,h} = 4\pi\,n\,M_{i,h,a}\,D_{\mathrm{sO_2}}\,([\mathrm{O_{2s}}] - [\mathrm{O}_{2\mathrm{m}i,h}])\,[r_\mathrm{m} r_\mathrm{w} / (r_\mathrm{w} - r_\mathrm{m})] \qquad \text{[H4a]}$$

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

$$X_{\mathrm{DOC}i,h} = X'_{\mathrm{DOC}i,h}\;R_{\mathrm{O_2}i,h} / R'_{\mathrm{O_2}i,h} \qquad \text{[H5]}$$

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

$$R'_{\mathrm{NO_3}i,d} = \boldsymbol{E}_{\mathbf{No_x}}\,(R'_{\mathrm{O_2}i,d} - R_{\mathrm{O_2}i,d})\,(1.0 + \boldsymbol{K}_\mathbf{e}\,(R'_{\mathrm{O_2}i,d} - R_{\mathrm{O_2}i,d})/V_i) \qquad \text{[H6]}$$

$$R_{\mathrm{NO_3}i,d} = R'_{\mathrm{NO_3}i,d}\,[\mathrm{NO_3^-}] / ([\mathrm{NO_3^-}] + \boldsymbol{K}_{\mathbf{NO_3}\boldsymbol{d}})\;/(1.0+([\mathrm{NO_2^-}]\,\boldsymbol{K}_{\mathbf{NO_3}\boldsymbol{d}})/(\,[\mathrm{NO_3^-}]\,\boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{d}})) \qquad \text{[H7]}$$

$$R_{\mathrm{NO_2}i,d} = (R'_{\mathrm{NO_3}i,d} - R_{\mathrm{NO_3}i,d})\,[\mathrm{NO_2^-}] / ([\mathrm{NO_2^-}] + \boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{d}})\;/(1.0+([\mathrm{N_2O}]\,\boldsymbol{K}_{\mathbf{NO2}\boldsymbol{d}})/(\,[\mathrm{NO_2^-}]\,\boldsymbol{K}_{\mathbf{N2O}\boldsymbol{d}})) \qquad \text{[H8]}$$

$$R_{\mathrm{N_2O}i,d} = 2\,(R'_{\mathrm{NO_3}i,d} - R_{\mathrm{NO_3}i,d} - R_{\mathrm{NO_2}i,d})\,[\mathrm{N_2O}] / ([\mathrm{N_2O}] + \boldsymbol{K}_{\mathbf{N_2O}\boldsymbol{d}}) \qquad \text{[H9]}$$

$$X_{\mathrm{DOC}i,d} = X_{\mathrm{DOC}i,d}\ (\text{from [H5]}) + \boldsymbol{F}_{\mathbf{NO_x}}\,(R_{\mathrm{NO_3}i,d} + R_{\mathrm{NO_2}i,d}) + \boldsymbol{F}_{\mathbf{N_2O}}\,R_{\mathrm{N_2O}i,d} \qquad \text{[H10]}$$

Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers

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

$$R'_{\mathrm{O_2}i,n} = \mathbf{RQ_{NH_3}}\,X'_{\mathrm{NH_3}i,n} + \mathbf{RQ_C}\,X'_{\mathrm{C}i,n} \qquad \text{[H12]}$$

$$R_{\mathrm{O_2}i,n} = 4\pi\,n\,M_{i,n,a}\,D_{\mathrm{sO_2}}\,(r_\mathrm{m}\,r_\mathrm{w} / (r_\mathrm{w} - r_\mathrm{m}))\,([\mathrm{O_{2S}}] - [\mathrm{O}_{2\mathrm{m}i,n}]) \qquad \text{[H13a]}$$

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

$$X_{\mathrm{NH_3}i,n} = X'_{\mathrm{NH_3}i,n}\,R_{\mathrm{O_2}i,n} / R'_{\mathrm{O_2}i,n} \qquad \text{[H14]}$$

Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers

$$X'_{\mathrm{NO_2}i,o} = X'_{\mathrm{NO_2}}\,M_{i,o,a}\;\{[\mathrm{NO_2^-}] / ([\mathrm{NO_2^-}] + \boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{o}})\}\;\{[\mathrm{CO_{2S}}] / ([\mathrm{CO_{2S}}] + \boldsymbol{K}_{\mathbf{CO_2}})\}\,f_\mathrm{t} \qquad \text{[H15]}$$

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

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

$$= R'_{O_2 i,o} \, [O_{2m i,o}] / ([O_{2m i,o}] + \boldsymbol{K}_{\mathbf{O_2}\boldsymbol{o}}) \qquad \text{[H17b]}$$

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

Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers

$$R'_{NO_2 i,n} = \boldsymbol{E}_{\mathbf{NO_x}} \, (R'_{O_2 i,n} - R_{O_2 i,n})/(1.0 + \boldsymbol{K}_{\mathbf{e}} \, (R'_{O_2 i,n} - R_{O_2 i,n})/V_i) \qquad \text{[H19]}$$

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

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

Definition of Variables in Section 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 $M_{i,m}$				
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 $M_{i,m,j,N}$ to $M_{i,m,j,C}$ maintained by $M_{i,m,j}$	g N g C^{-1}	[H1]	0.22 and 0.13 for *j* = labile and resistant	
$[CO_{2S}]$	CO_2 concentration in soil solution	g C m^{-3}	[H11,H15,H20]		
$[DOC_i]$	concentration of dissolved decomposition products	g C m^{-3}	[H2]		
D_{sO_2}	aqueous dispersivity-diffusivity of O_2	m^2 h^{-1}	[H4,H13,H17]		
$\boldsymbol{E}_{\mathbf{NO_x}}$	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	
f_t	temperature function for microbial processes	-	[H2,H11,H15]		See SectionA
$I_{NH_4 i,n,j}$	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]	0.0002	Suzuki et al. (1974)
$\boldsymbol{Ke}$	inhibition constant for electrons not accepted by O_2 and transferred to N oxides	-	[H6,H19]	0.5	from Koike and Hattori (1975)
$\boldsymbol{K}_{\mathbf{NH_4}\boldsymbol{m}}$	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	$g\ N\ m^{-3}$	[H7,H8]	1.4	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]	1.4	
$\boldsymbol{K}_{\mathbf{NO_2}\boldsymbol{o}}$	M-M constant for oxidation of NO_2^- by nitrifiers	$g\ N\ m^{-3}$	[H15]	3.5	
$\boldsymbol{K}_{\mathbf{NO_3}\boldsymbol{d}}$	M-M constant for reduction of NO_3^- by denitrifiers	$g\ N\ m^{-3}$	[H7,H8]	1.4	Yoshinari et al. (1977);Khalil et al., 2005
$\boldsymbol{K}_{\mathbf{N_2O}\boldsymbol{d}}$	M-M constant for reduction of N_2O by denitrifiers	$g\ N\ m^{-3}$	[H9]	0.028	Yoshinari et al. (1977);Khalil et al., 2005
$\boldsymbol{K}_{\mathbf{O_2}\boldsymbol{h}}$	M-M constant for reduction of O_{2s} by heterotrophs	$g\ O_2\ m^{-3}$	[H4b]	0.064	Griffin (1972)
$\boldsymbol{K}_{\mathbf{O_2}\boldsymbol{n}}$	M-M constant for reduction of O_{2s} by NH_3 oxidizers	$g\ O_2\ m^{-3}$	[H13b]	0.064	Focht and Verstraete (1977)

$\boldsymbol{K_{O_2 o}}$	M-M constant for reduction of O_{2s} by NO_2^- oxidizers	g O_2 m^{-3}	[H17b]	0.064	Focht and Verstraete (1977)
$\boldsymbol{K_{Xh}}$	M-M constant for oxidation of DOC by heterotrophs	g C m^{-3}	[H2]	12	(McGill et al., 1981)
$M_{i,h,a}$	active biomass of heterotrophs	g C m^{-2}	[H2,H7]		
$M_{i,n,a}$	active biomass of NH_3 oxidizers	g C m^{-2}	[H11,H13]		
$M_{i,m,j,\mathrm{C}}$	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}	[H7,H8,H15,H20]		
$[NO_3^-]$	concentration of NO_3^- in soil solution	g N m^{-3}	[H7,H8]		
$[N_2O]$	concentration of N_2O in soil solution	g N m^{-3}	[H9]		
n	number of microbes	g^{-1}	[H13,H17]		
$[O_{2mi,h}]$	O_2 concentration at heterotrophic surfaces	g O_2 m^{-3}	[H7]		
$[O_{2mi,n}]$	O_2 concentration at NH_3 oxidizer surfaces	g O_2 m^{-3}	[H13]		
$[O_{2mi,o}]$	O_2 concentration at NO_2^- oxidizer surfaces	g O_2 m^{-3}	[H17]		
$[O_{2s}]$	O_2 concentration in soil solution	g O_2 m^{-3}	[H7,H13,H17]		
$R_{NO_2 i,d}$	NO_2^- reduction by denitrifiers	g N m^{-2} h^{-1}	[H8,H9,H10]		
$R'_{NO_2 i,n}$	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]		

$R_{\mathrm{O}_2 i,d}$	rate of O_{2S} reduction by denitrifiers under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H6]		
$R'_{\mathrm{O}_2 i,h}$	rate of O_{2S} reduction by heterotrophs under non-limiting $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H3,H4,H5]		
$R_{\mathrm{O}_2 i,h}$	rate of O_{2S} reduction by heterotrophs under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H4,H5]		
$R'_{\mathrm{O}_2 i,n}$	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 O_{2S} reduction by NH_3 oxidizers under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H13,H14,H19]		
$R'_{\mathrm{O}_2 i,o}$	rate of O_{2S} reduction by NO_2^- oxidizers under non-limiting $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H16,H17,H18]		
$R_{\mathrm{O}_2 i,o}$	rate of O_{2S} reduction by NO_2^- oxidizers under ambient $[O_{2S}]$	$g\ O_2\ m^{-2}\ h^{-1}$	[H17,H18]		
$\mathbf{RQ_C}$	respiratory quotient for reduction of O_2 coupled to oxidation of C	$g\ O_2\ g\ C^{-1}$	[H3,H12,H16]	2.67	Brock and Madigan (1991)
$\mathbf{RQ_{NH_3}}$	respiratory quotient for reduction of O_2 coupled to oxidation of NH_{3S}	$g\ O_2\ g\ N^{-1}$	[H12]	3.43	Brock and Madigan (1991)
$\mathbf{RQ_{NO_2}}$	respiratory quotient for reduction of O_2 coupled to oxidation of NO_2^-	$g\ O_2\ g\ N^{-1}$	[H16]	1.14	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)
V_i	soil volume occupied by substrate-microbe complex		[H6,H19]		
$X'_{\mathrm{C}i,n}$	rate of C oxidation by NH_3 oxidizers under non-limiting $[O_{2S}]$	$g\ C\ m^{-2}\ h^{-1}$	[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 $[O_{2S}]$	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 $[O_{2S}]$	g N m^{-2} h^{-1}	[H18]		
$X'_{\mathrm{NO_2}}$	specific rate of NO_2^- oxidation by NO_2^- oxidizers at 25 °C under non-limiting $[O_{2S}]$	g N g C^{-1} h^{-1}	[H15]	2.5	Belser (1977)

References

Addiscott, T.M. 1983. Kinetics and temperature relationships of mineralization and nitrification in Rothamsted soils with differing histories. Journal of Soil Science 34:343-353.

Anthony, C. 1982. *The Biochemistry of Methylotrophs*. Academic Press. London, U.K.

Barber, S.A. and M. Silberbush. 1984. Plant root morphology and nutrient uptake. pp. 65-87. *In* S.A. Barber and D.R. Bouldin (eds.). Roots, Nutrient and Water Influx, and Plant Growth. Amer. Soc. Agron. Spec. Publ. no. 49. Madison, WI.

Barnes, B.V., D.R. Zak, S.R. Denton and S.H. Spurr. 1998. Forest Ecology 4th ed. Wiley and Sons. N.Y.

Belser, L.W. 1977. Nitrate reduction to nitrite, a possible source of nitrite for growth of nitrite-oxidizing bacteria. Appl. Environ. Micro. 34:403-410.

Belser, L.W. and E.L. Schmidt. 1980. Growth and oxidation kinetics of the three genera of ammonia oxidizers. FEMS Microbiol. Lett. 7:213-216.

Bernacchi, C.J., E.L. Singsaas, C. Pimentel, A.L. Portis and S.P. Long. 2001. Improved temperature response functions for models of rubisco-limited photosynthesis. Plant, Cell and Environment 24:253-259.

Bernacchi, C.J., C. Pimentel. and S.P. Long. 2003. In vivo temperature response functions of parameters required to model RuBP-limited photosynthesis. Plant, Cell and Environment 26:1419–1430.

Berry J.A. and G.D. Farquhar. 1978. The CO2 concentrating function of photosynthesis: a biochemical model. pp. 119-131 In: Proceedings of the 4th Interntl. Congress on Photosynthesis. Hall D., Coombs J. and Goodwin T. eds. Biochemical Society. London.

Brock, T.D. and Madigan, M.T. 1991. *Biology of Microorganisms* (6th. Ed.). Prentice Hall, NJ.

Campbell, G.S. 1985. Soil Physics with BASIC. Elsevier, Netherlands. 185 pp.

Chowdhury, N., Marschner, P. and Burns, R.G. 20011. Soil microbial activity and community composition: Impact of changes in matric and osmotic potential. . Soil Biology & Biochemistry 43:1229-1236.

Conrad, R. 1984. Capacity of aerobic microorganisms to utilize and grow on atmospheric trace gases (H_2, CO, CH_4). In *Current Perspectives in Microbial Ecology*. Klug M.J. and Reddy C.A. (eds). Amer. Soc. Microbiol. Wash. DC. pp. 461-467.

de Vries, D.A. 1963. Thermal properties of soils. pp 210-235 In: van Wijk, R. (ed). *Physics of Plant Environment*. North Holland Publishing Co. Amsterdam, Netherlands

Dimitrov, D.D., Grant, R.F., LaFleur, P.M. and Humphreys, E. 2010. Modelling subsurface hydrology of Mer Bleue bog. Soil Science Society of America Journal 74:680-694 .

Doussan C., G. Vercambre and L. Pagès. 1998. Modelling of the hydraulic architecture of root systems: An integrated approach to water absorption – distribution of axial and radial conductances in maize. Annals of Botany 81:225-232.

Edwards, G. and D. Walker. 1983. C3, C4: Mechanisms, and Cellular and Environmental Regulation of Photosynthesis. Univ. of California Press, Berkely CA.

Farquhar G.D., S. von Caemmerer and J.A. Berry. 1980. A biochemical model of photosynthetic CO_2 assimilation in leaves of C_3 species. Planta 149:78-90.

Focht, D.D. and W. Verstraete.1977. Biochemical ecology of nitrification and denitrification. Adv. Micro. Ecol. 1:135-214.

Furbank, F.T. and M.D. Hatch. 1987. Mechanism of C4 photosynthesis. The size and composition of the inorganic carbon pool in bundle sheath cells. Plant Physiol. 85:958-964.

Grant, R.F. 1995. Mathematical modelling of nitrous oxide evolution during nitrification. *Soil Biology & Biochemistry* **27**, 1117-1125.

Grant, R.F. 1998. Simulation in *ecosys* of root growth response to contrasting soil water and nitrogen Ecological Modelling 107: 237-264.

Grant, R.F. 1998b. Simulation of methanogenesis in the mathematical model *ecosys*. *Soil Biology & Biochemistry* **30**,883-896.

Grant, R.F. 1999. Simulation of methanotrophy in the mathematical model *ecosys*. *Soil Biology & Biochemistry* **31**, 287-297.

Grant, R.F. 2004. Modelling topographic effects on net ecosystem productivity of boreal black spruce forests. Tree Physiol. 24:1-18.

Grant, R.F. 2001. A review of the Canadian ecosystem model *ecosys*. pp. 173-264 in: Modeling Carbon and Nitrogen Dynamics for Soil Management. Shaffer M. (ed). CRC Press. Boca Raton, FL

Grant, R.F. and Hesketh, J.D. 1992. Canopy structure of maize *(Zea mays L.)* at different populations: simulation and experimental verification. *Biotronics.* 21: 11-24.

Grant, R.F. and Rochette, P. 1994. Soil microbial respiration at different temperatures and water potentials: Theory and mathematical modelling. *Soil Science Society of America Journal* **58**, 1681-1690.

Grant, R.F., M. Amrani, D.J. Heaney, R. Wright and M. Zhang. 2004. Mathematical modelling of phosphorus losses from land application of hog and cattle manure. Journal of Environmental Quality 33:210-233.

Grant, R.F., T.A. Black, E.R. Humphreys, and K. Morgenstern. 2007. Changes in net ecosystem productivity with forest age following clearcutting of a coastal Douglas fir forest: testing a mathematical model with eddy covariance measurements along a forest chronosequence. Tree Physiology. 27:115-131.

Grant, R. F. and L. B. Flanagan. 2007. Modeling stomatal and nonstomatal effects of water deficits on CO_2 fixation in a semiarid grassland. Journal of Geophysical Research 112:G03011, doi:10.1029/2006JG000302.

Grant, R.F. and D.J. Heaney. 1997. Inorganic phosphorus transformation and transport in soils: mathematical modelling in *ecosys*. Soil Science Society of America Journal 61:752-764.

Grant, R.F., N.G. Juma, and W.B. McGill. 1993a. Simulation of carbon and nitrogen transformations in soils. I. Mineralization. Soil Biology & Biochemistry 27:1317–1329.

Grant, R.F., N.G. Juma, and W.B. McGill. 1993b. Simulation of carbon and nitrogen transformations in soils. II. Microbial biomass and metabolic products. Soil Biology & Biochemistry 27:1331–1338.

Grant, R.F., G.W. Wall, B.A. Kimball, K.F.A. Frumau, P.J. Pinter Jr., D.J. Hunsaker, and R.L. Lamorte. 1999. Crop water relations under different CO_2 and irrigation: testing of ecosys with the free air CO_2 enrichment (FACE) experiment. Agricultural & Forest Meteorology 95:27-51.

Grant, R.F., B.A. Kimball, G.W. Wall, J.M. Triggs, T.J. Brooks, P.J. Pinter Jr., M.M. Conley, M.J. Ottman, R.L. Lamorte, S.W. Leavitt, T.L. Thompson and A.D. Matthias. 2004. How elevated CO2 affects water relations, water use and growth of irrigated sorghum: testing a model with results from a Free Air CO2 Enrichment (FACE) experiment Agron. J. 96: 1693-1705.

Grant, R.F., Barr, A.G., Black, T.A., Margolis, H.A., McCaughey, J.H. and Trofymow, J.A. 2010. Net ecosystem productivity of temperate and boreal forests after clearcutting – a Fluxnet-Canada synthesis. *Tellus B.* 62B: 475-496.

Green, R.E., and R.B. Corey. 1971. Calculation of hydraulic conductivity: A further evaluation of some predictive methods. Soil Sci. Soc. Am. Proc. 35:3–8.

Griffin, D.M. 1972. Ecology of Soil Fungi. Syracuse Univ. Press, Syracuse N.Y. 193 pp.

Jiao, J.A. and R. Chollet. 1988. Light/dark regulation of maize leaf phosphoenol pyruvate carboxylase by in vivo phosphorylation. Arch. Biochem. Biophys. 261:409-417.

Kemper, W.D. and J.B. Rollins. 1966. Osmotic efficiency coefficients across compacted clays. Soil Sci. Soc. Amer. Proc. 30:529-534.

Khalil, K., P. Renault, N. Guérin and B. Mary. 2005. Modelling denitrification including the dynamics of denitrifiers and their progressive ability to reduce nitrous oxide: comparisonwith batch experiments. Euro. J. Soil Sci. 56:491–504.

Kimmins, J.P. 2004. Forest Ecology. Pearson Prentice Hall, NJ.

Koike, I. and A. Hattori. 1975. Growth yield of a denitrifying bacterium, *Pseudomonas denitrificans*, under aerobic and denitrifying conditions. J. Gen. Microbiol. 88:1-10.

Laisk, A. and G.E. Edwards. 2000. A mathematical model of C4 photosynthesis: The mechanism of concentrating CO2 in NADP – malic enzyme type species. Photosyn. Res. 66:199-224.

Larcher, W. 2001. Physiological Plant Ecology 4th ed. Springer-Verlag. Berlin

Lawlor, D. 1993. Photosynthesis: molecular, physiological and environmental processes. Longman Group, Essex, UK.

Lawrence A.L. 1971. Anaerobic biological treatment processes. In Advances in Chemistry Series 105. Gould R.F. (ed.). Amer. Chem. Soc. Wash. D.C. pp. 163-189.

Leegood, R.C. 2000. Transport during C4 photosynthesis. pp. 449-469. In Advances in Photosynthesis: 9. Photosynthesis: Physiology and Metabolism. Leegood, R.C., Sharkey, T.D. and von Caemmerer, S. (eds). Kluwer Academic Publishers, Dordrecht.

Lizama H.M. and Suzuki I. 1990. Kinetics of sulfur and pyrite oxidation by *Thiobacillus thiooxidans*. Competitive inhibition by increasing concentrations of cells. Canadian Journal of Microbiology 37, 182-187.

Luxmoore R.J., L.H. Stolzy and J. Letey. 1970a Oxygen diffusion in the soil-plant system. I. a model. Agron. J. 62, 317-322.

Luxmoore R.J., L.H. Stolzy and J. Letey. 1970b Oxygen diffusion in the soil-plant system. II. respiration rate, permeability, and porosity of consecutive excised segments of maize and rice roots. Agron. J. 62, 322-324.

McGill W.B., Hunt H.W., Woodmansee R.G. and Reuss J.O. (1981) Phoenix, a model of the dynamics of carbon and nitrogen in grassland soils. In Terrestrial Nitrogen Cycles. (F.E. Clark and T. Rosswall eds) Ecological Bulletins 33, 49-115.

Medrano, H., J.M. Escalona, J. Bota, J. Gulías and J. Flexas, Regulation of photosynthesis of C_3 plants in response to progressive drought: stomatal conductance as a reference parameter. *Ann. Bot*., *89*, 895-905, 2002.

Mosey F.E. 1983. Kinetic descriptions of anaerobic digestion. In *Third International Symposium on Anaerobic Digestion* Boston Univ. Cambridge, MS. pp. 37-52.

Millington, R.J. and J.M. Quirk. 1960. Transport in porous media. pp. 97-106 In: Van Beren, F.A. et al. (eds). 7th Trans. Int. Congr. Soil Sci. vol. 1. Madison, WI. 14-24 Aug. 1960. Elsevier, Amsterdam.

Perrier, A. 1982. Land surface processes: vegetation. pp. 395-448 In: *Atmospheric General Circulation Models.* Eagleson P.S. (ed.). Cambridge Univ. Press. Cambridge, U.K.

Pirt S.J. 1975. Principles of Microbe and Cell Cultivation. Blackwell Scientific. Oxford, U.K.

Postgate, J. 1998. Nitrogen Fixation (3rd Ed.). Cambridge Univ. Press, Cambridge, UK. 112 pp.

Robinson J.A. and Tiedje J.M. 1982. Kinetics of hydrogen consumption by rumen fluid, digestor sludge and sediment. *Applied and Environmental Microbiology* **44**, 1374-1384.

Sawada, S., T. Sakamoto, M. Sato, M. Kasai and H. Usuda. 2002. Photosynthesis with single-rooted Amaranthus leaves. II. Regulation of Ribulose-1,5-Bisphosphate Carboxylase, Phosphoenolpyruvate Carboxylase, NAD-Malic Enzyme and NAD-Malate Dehydrogenase and coordination between PCR and C4 photosynthetic metabolism in response to changes in the source-sink balance. Plant Cell Physiol. 43(11):1293-301.

Schink B. 1997. Energetics of syntrophic cooperation in methanogenic degradation. *Microbiology and Molecular Biology Reviews*. **61**, 262-280.

Seeman, J.R., M.R. Badger and J.A. Berry. 1984. Variations in the specific activity of ribulose-1,5-bisphosphate carboxylase between species utilizing differing photosynthetic pathways. Plant Physiol. 74:791-794.

Sharpe, P.S.H. and D.W. DeMichelle. 1977. Reaction kinetics of poikilothermic development. Journal of Theoretical Biology 64:649-670.

Shea T.G., Pretorius W.E., Cole R.D. and Pearson E.A. 1968. Kinetics of hydrogen assimilation in the methane fermentation. *Water Research* **2**, 833-848.

Shields J.A., E.A. Paul, W.E. Lowe and D. Parkinson. 1973. Turnover of microbial tissue in soil under field conditions. Soil Biology & Biochemistry 5:753-764.

Shulten, H.-R., and M. Schnitzer. 1997. Chemical model structures for organic matter and soils. Soil Science 162:115–130.

Skopp, J. 1985. Oxygen uptake and transfer in soils: analysis of the air-water interfacial area. Soil Sci. Soc. Amer. J. 49:1327-1331.

Smith M.R. and Mah R.A. 1978. Growth and methanogenesis by *Methanosarcina* strain 227 on acetate and methanol. *Applied & Environmental Microbiology* **36**, 870-879.

Sørenson L.H. (1981) Carbon-nitrogen relationships during the humification of cellulose in soils containing different amounts of clay. *Soil Biology & Biochemistry* **13**, 313-321.

Suzuki, I., U. Dular and S.C. Kwok. 1974. Ammonia or ammonium ion as substrate for oxidation by *Nitrosomonas europeae* cells and extracts. J. Bacteriol. 120:556-558.

van Bavel, C.H.M., and D.I. Hillel. 1976. Calculating potential and actual evaporation from a bare soil surface by simulation of concurrent flow of water and heat. Agric. Meteorol. 17:453-476.

Veen, B.W. 1981. Relation between root respiration and root activity. Plant Soil 63: 73-76.

Waring, R.H. and S.W. Running. 1998. Forest Ecosystems: Analysis at Multiple Scales. (2nd ed.) Academic Press. London U.K.

Wilhelm, E., R. Battino and R.J. Wilcock. 1977. Low-pressure solubility of gases in liquid water. Chem. Rev. 77:219-262.

Williams D.G., V. Gempko, A. Fravolini, S.W. Leavitt, G.W. Wall, B.A. Kimball, P.J. Pinter Jr., R. LaMorte and M. Ottman. 2001. Carbon isotope discrimination by Sorghum bicolor under CO2 enrichment and drought. New Phytol. 150:285-293.

Wofford N.G., Beaty P.S. and McInerey M.J. 1986. Preparation of cell-free extracts and the enzymes involved in fatty acid metabolism in *Syntrophomonas wolfei*. *Journal of Bacteriology* **167**, 189-195.

Yoshinari. T., R. Hynes and R. Knowles. 1977. Acetylene inhibition of nitrous oxide reduction and measurement of denitrification and nitrogen fixation in soil. Soil Biol. Biochem. 9:177-183.

Zehnder A.J.B. and Wuhrmann K. 1977. Physiology of a *Methanobacterium* strain AZ. *Archives of Microbiology* **111**, 199-205.

Zehnder A.J.B., Huser B.A., Brock T.D. and Wuhrmann K. 1980. Characterization of an acetate-decarboxylating, non-hydrogen-oxidizing methane bacterium. *Archives of Microbiology* **124**, 1-11.