Supplement of

Ecological controls on $\text{N}_2\text{O}$ emission in surface litter and near-surface soil of a managed grassland: modelling and measurements

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SUPPLEMENTARY MATERIAL

Model Development

General

Ecosys is an hourly time-step model with multiple canopy and soil layers that provide a framework for simulated plant and microbial populations to acquire, transform and exchange resources (energy, water, C, N and P). The model is constructed from algorithms representing basic physical, chemical and biological processes that determine process rates in plant and microbial populations interacting within complex biomes. These algorithms interact to simulate complex ecosystem behaviour across a wide range of spatial and biological scales. The model is designed to represent terrestrial ecosystems under range of natural and anthropogenic disturbances and environmental changes at patch (spatially homogenous one-dimensional) and landscape (spatially variable two- or three-dimensional) scales. A comprehensive description of ecosys with a detailed listing of inputs, outputs, governing equations, parameters, results and references can be found in Grant (2001). A more detailed description of model algorithms and parameters most relevant to simulating temperature, water and nutrient effects on NEP is given below, with reference to equations and variable definitions in 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 \( (\theta) \) through its effect on aqueous microbial concentrations \( [M] \) [A3, A5] in surface litter and in a spatially resolved soil profile. \( T_s \) and \( \theta \) are calculated from surface energy balances and from heat and water transfer schemes through canopy–snow–residue–soil profiles as described in Energy
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\(_2\)O by heterotrophic denitrifiers, and with the reduction of organic C by fermenters and acetotrophic methanogens. In addition, autotrophic nitrifiers conduct NH\(_4^+\) and NO\(_3^-\) oxidation, and NO\(_2^-\) reduction, and autotrophic methanogens and methanotrophs conduct CH\(_4\) production and oxidation.

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

**Microbial Nutrient Exchange**

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

C3 Gross Primary Productivity

After successful convergence for \(T_c\) and \(\psi_c\) (described in Plant Water Relations above), \(V_c\) is recalculated from that under zero \(\psi_c\) \((V'_c)\) to that under ambient \(\psi_c\). This recalculation is driven by stomatal effects on \(V_g\) \((C2)\) from the increase in \(r_{\text{min}}\) at zero \(\psi_c\) \((C5)\) to \(r_c\) at ambient \(\psi_c\) \((C4)\), and by non-stomatal effects \(f_{\psi}\) \((C9)\) 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 \(\sigma_c\) in each branch.

GPP is strongly controlled by nutrient uptake \(U_{\text{NH}_4}, U_{\text{NO}_3}\) and \(U_{\text{PO}_4}\) \([C23]\), products of which are added to nonstructural N \((\sigma_N)\) and P \((\sigma_P)\) in root and mycorrhizal layers where they are coupled with \(\sigma_c\) to drive growth of branches, roots and mycorrhizae as described in Growth and Senescence below. Low \(\sigma_N:\sigma_c\) or \(\sigma_P:\sigma_c\) in branches indicate excess CO\(_2\) fixation with respect to N or P uptake for phytomass growth. Such ratios in the model have two effects on GPP:

1. They reduce activities of rubisco \([C6a]\) and chlorophyll \([C7a]\) through product inhibition \([C11]\), thereby simulating the suppression of CO\(_2\) fixation by leaf \(\sigma_c\) accumulation widely reported in the literature.
2. They reduce the structural N:C and P:C ratios at which leaves are formed because \(\sigma_c, \sigma_N\) and \(\sigma_P\) are the substrates for leaf growth. Lower structural ratios cause a proportional reduction in areal concentrations of rubisco \([C6b]\) and chlorophyll \([C7b]\), reducing leaf CO\(_2\) fixation.

Autotrophic Respiration

The temperature-dependent oxidation of these nonstructural pools \((R_a)\) \([C14]\), plus the energy costs of nutrient uptake \([C23]\), drive autotrophic respiration \((R_a)\) \([C13]\) by all branches, roots and mycorrhize. \(R_c\) by roots and mycorrhizae is constrained by O\(_2\) uptake \(U_{O_2}\) \([C14b]\) calculated by solving for aqueous O\(_2\) concentrations at root and
mycorrhizal surfaces \([O_2]\) 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 \(\psi_t\) \([C17]\). When \(R_m\) exceeds \(R_c\), the shortfall is met by the respiration of remobilizable \(C\) \((R_c)\) in leaves and twigs or roots and mycorrhizae \([C15]\).

**Growth and Litterfall**

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

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

\(R_g\) is limited by \(\psi_t\) \([C17]\), and because branch \(\psi_t\) declines relatively more with soil drying than does root \(\psi_r\), branch \(R_g\) also declines relatively more with soil drying than...
does root $R_g$, slowing oxidation of $\sigma_C$ in branches and allowing more translocation of $\sigma_C$ from branches to roots. This change in allocation of $\sigma_C$ enables more root growth to reduce $\Omega_s$, $\Omega_t$ and $\Omega_a$, and hence increase $U$ [B6], thereby offsetting the effects of soil drying on $\psi$. Thus the modelled plant translocates $\sigma_C$, $\sigma_N$ and $\sigma_P$ among branches, roots and mycorrhizae to maintain a functional equilibrium between acquisition and use of water.

$R_s$ [C15] drives the withdrawal of remobilizable C, N and P (mostly nonstructural protein) from leaves and twigs or roots and mycorrhizae into $\sigma_N$ and $\sigma_P$, and the loss of associated non-remobilizable C, N and P (mostly structural) as litterfall [C18, C19a,b]. Provision is also made to withdraw remobilizable N or P from leaves and twigs or roots and mycorrhizae when ratios of $\sigma_N$:$\sigma_C$ or $\sigma_P$:$\sigma_C$ become smaller than those required for growth of new phytomass [C19c,d]. This withdrawal drives the withdrawal of associated remobilizable C, and the loss of associated non-remobilizable C, N and P as litterfall.

Environmental constraints such as water, heat, nutrient or O$_2$ stress that reduce $\sigma_C$ and hence $R_c$ with respect to $R_m$ therefore hasten litterfall. In addition, concentrations of $\sigma_C$, $\sigma_N$ and $\sigma_P$ in roots and mycorrhizae drive exudation of nonstructural C, N and P to DOC, DON and DOP in soil [C19e-i].

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

**Root and Mycorrhizal Nutrient Uptake**

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

**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], $\psi_c$ ([C35] as described in Grant and Flanagan, 2007) and $T_c$ [C10]. Leaf surface N density is controlled by leaf structural N:C and P:C ratios calculated during leaf growth from leaf non-structural N:C and P:C ratios arising from root N and P uptake (Grant, 1998) vs. CO$_2$ 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], $\psi_c$ (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\textsubscript{3} carboxylation [C43], raise bundle sheath CO\textsubscript{2} concentration [C42], accelerate CO\textsubscript{2} leakage [C39], slow C\textsubscript{4} decarboxylation [C38], raise C\textsubscript{4} product concentration in the bundle sheath [C41], slow C\textsubscript{4} product transfer from the mesophyll [C37], raise C\textsubscript{4} product concentration in the mesophyll [C40], and slow mesophyll CO\textsubscript{2} fixation [C32 – C35]. This reaction sequence simulates the progressive inhibition of C\textsubscript{3} and C\textsubscript{4} carboxylation hypothesized by Sawada et al. (2002) following partial removal of C sinks in C\textsubscript{4} plants.

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

Shoot – root C transfers \(Z_{C}\) are calculated such that concentrations of \(\sigma_{C}\) with respect to structural phytomass in each branch and root layer approach equilibrium according to conductances \(g_{C}\) calculated from shoot – root distances and axis numbers in each root layer [C50] (Grant, 1998). Because \(\sigma_{C}\) is generated by CO\textsubscript{2} fixation in branches [C1], \(g_{C}\) cause shoot-to-root gradients of \(\sigma_{C}\) that drive \(Z_{C}\). Shoot – root N and P transfers \(Z_{N,P}\) are calculated such that concentrations of \(\sigma_{N,P}\) with respect to \(\sigma_{C}\) in each branch and root layer approach equilibrium according to rate constants \(g_{N,P}\) [C51]. Because \(\sigma_{N,P}\) are generated by uptake in roots [C23], \(g_{N,P}\) cause root-to-shoot gradients of \(\sigma_{N,P}\) that drive \(Z_{N,P}\).

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

**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 \(\psi_{s}\) of both cells if both source and destination cells are unsaturated [D9a], or Green-Ampt equation using \(\psi_{s}\) beyond the wetting front of the unsaturated cell if either source or destination cell is saturated [D9b] (Grant et al., 2004). Subsurface
water flow can also occur through macropores using 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 \([\text{NH}_4^+]\), \([\text{NO}_3^-]\) and \([\text{H}_2\text{PO}_4^-]\) that drive \(U_{\text{NH}_4}\), \(U_{\text{NO}_3}\) and \(U_{\text{PO}_4}\) [C23] are controlled by precipitation, adsorption and ion pairing reactions (Grant et al., 2004; Grant and Heaney, 1997), including precipitation-dissolution of \(\text{Al(OH)}_3\), \(\text{Fe(OH)}_3\), \(\text{CaCO}_3\), \(\text{CaSO}_4\), \(\text{AlPO}_4\), \(\text{FePO}_4\), \(\text{Ca(H}_2\text{PO}_4)_2\), \(\text{CaHPO}_4\), and \(\text{Ca}_5(\text{PO}_4)_3\text{OH}\) [E1 – E9], cation
exchange between Ca\(^{2+}\), NH\(_4^+\) and other cations [E10 – E15], anion exchange between adsorbed and soluble H\(_2\)PO\(_4^-\), 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 \(j\) \((j = \text{labile or resistant})\) of each microbial population \(m\) \((m = \text{obligately aerobic bacteria, obligately aerobic fungi, facultatively anaerobic denitrifiers, anaerobic fermenters plus H}_2\text{-producing acetogens, acetotrophic methanogens, hydrogenotrophic methanogens and methanotrophs, NH}_4^+\text{ and NO}_2^-\text{ oxidizers, and non-symbiotic diazotrophs})\) in each substrate-microbe complex \(i\) \((i = \text{animal manure, coarse woody plant residue, fine non-woody plant residue, particulate organic matter, or humus})\) 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$_2$O,
4) N$_2$O reduction under ambient N$_2$O 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$_2$ oxidation 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

\[ D_{S_{i,j},C} = D'_{S_{i,j},C} M_{i,d,l,c} f_{ig} (S_{i,j,C} / G_{i,l,C}) \]
\[ D_{Z_{i,j},C} = D'_{Z_{i,j},C} M_{i,d,l,c} f_{ig} (Z_{i,l,C} / G_{i,l,C}) \]
\[ D_{A_{i,j},C} = D'_{A_{i,j},C} M_{i,d,l,c} f_{ig} (A_{i,j,C} / G_{i,l,C}) \]
\[ S_{i,l,C} = \Sigma_i S_{i,j,l,C} \]
\[ Z_{i,l,C} = \Sigma_i Z_{i,j,l,C} \]
\[ G_{i,l,C} = S_{i,l,C} + Z_{i,l,C} + A_{i,l,C} \]
\[ M_{i,d,l,C} = M_{i,a,l,C} + q_m (M_{i,a,l,C} G_{i,l,C} - M_{i,a,l,C} G_{i,l,C}) / (G_{i,l,C} + G_{i,l,C}) \]
\[ M_{i,a,l,c} = \Sigma_n M_{i,n,a,l,c} \]
\[ D'_{S_{i,j},C} = \{D_{S_{i,l,C}} [S_{i,j,l,C}] / \{[S_{i,j,l,C}] + K_{\text{mD}} (1.0 + [\Sigma M_{i,a,l,C}] / K_{\text{mD}})\} \]
\[ D'_{Z_{i,j},C} = \{D_{Z_{i,l,C}} [Z_{i,j,l,C}] / \{[Z_{i,j,l,C}] + K_{\text{mD}} (1.0 + [M_{i,d,l,C}] / K_{\text{mD}})\} \]
\[ D'_{A_{i,j},C} = \{D_{A_{i,l,C}} [A_{i,l,C}] / \{[A_{i,l,C}] + K_{\text{mD}} (1.0 + [M_{i,d,l,C}] / K_{\text{mD}})\} \]
\[ \delta S_{i,j,l,C} / \delta t = \beta \Sigma_i (U_{i,n,C} - R_{\text{hi,n},i}) (S'_{i,j,k,l,C} / S_{i,j,l,C}) \{S'_{i,j,l,C} / S_{i,j,l,C} + K_{\text{hi}}\} \]
\[ f_{ig} = T_{a_d} (e^{[H - T_a / (R T_a)]} / \{1 + e^{(H - T_{a_d} - S T_{a_d}) / (R T_{a_d})} + e^{(S T_{a_d} - H_{a_d}) / (R T_{a_d})}\} \]

decomposition of litter, POC, humus
decomposition of microbial residues
decomposition of adsorbed SOC
total C in all kinetic components of litter, POC, humus
total C in all kinetic components of microbial residues
total C in substrate-microbe complexes
redistribution of active microbial biomass populations from each substrate-microbe complex to other substrate-microbe complexes according to concentration differences (priming)
substrate and water constraint on D from colonized litter, POC and humus, microbial residues and adsorbed SOC
colonized litter increases with microbial growth into uncolonized litter
Arrhenius function for D and R_h

[A1a] [A1b] [A1c] [A2a] [A2b] [A2c] [A3a] [A3b] [A4a] [A4b] [A4c] [A5] [A6]
\[ D_{S,i,l,NP} = D_{S,i,l,IC} (S_{i,l,NP} / S_{i,l,IC}) \]

\[ D_{Z,i,l,NP} = D_{Z,i,l,IC} (Z_{i,l,NP} / Z_{i,l,IC}) \]

\[ D_{A,i,l,NP} = D_{A,i,l,IC} (A_{i,l,NP} / A_{i,l,IC}) \]

\[ Y_{i,l,IC} = k_{u} (G_{i,l,IC} F_{i} [Q_{i,l,IC}]^{b} - X_{i,l,IC}) \]

\[ Y_{i,l,NP} = Y_{i,l,IC} (Q_{i,l,NP} / Q_{i,l,IC}) \]

\[ Y_{i,l,NP} = Y_{i,l,IC} (X_{i,l,NP} / X_{i,l,IC}) \]

**Microbial Growth**

\[ R_{h} = \sum \Sigma_{n} \sum_{l} R_{h,n,l} \]

\[ R_{h,n,l} = R'_{h,n} \min \{ C_{N_{i,n,l},a} / C_{N_{i}, C_{P_{u,n,l,a}} / C_{P_{l}}} \} \]

\[ R'_{h,n,l} = M_{n,n,a,l,IC} \{ R_{u,n,l} [Q_{i,l,IC}] / \{ (K_{m,c} + [Q_{i,l,IC}]) \} f_{qgl} / f_{egl} \]  

\[ R_{u,n,l} = R_{h,n,l} (U_{O2,n,l} \{ U'_{O2,n,l} \}) \]

\[ f_{qgl} = e^{(\sigma_{qgl})} \]

\[ U'_{O2,n,l} = 2.67 R_{h,n,l} \]

\[ U_{O2,n,l} = U'_{O2,n,l} [O_{2u,m,l,}] / \{ [O_{2u,m,l,}] + K_{O2} \} \]

\[ = 4 \pi n M_{n,n,a,l,IC} D_{a,2} [r_{m} (r_{m} / (r_{m} - r_{m})) (O_{2u,m,l,}) - [O_{2u,m,l,}] \]

\[ R_{u,n,l} = R_{u,n,l} M_{n,n,a,l,IC} f_{ml} \]

\[ f_{ml} = e^{(\sigma_{ml}) (r_{l} / 298.16)} \]

\[ R_{g,n,l} = R_{h,n,l} - \Sigma_{j} R_{m,j,n,l} \]

\[ U_{i,n,IC} = \min (R_{h,n,l} \Sigma_{j} R_{m,j,n,l}) + R_{g,n,l} (1 + \Delta G_{s} / E_{m}) \]

decomposition of N and P are driven by that of C in litter, POC, humus, microbial residues and adsorbed SOC

Freundlich sorption of DOC

\[ (Y_{i,l,IC} > 0) \]

adsorption of DON, DOP

\[ (Y_{i,l,IC} < 0) \]

desorption of DON, DOP

total heterotrophic respiration

\[ R_{h} \text{ constrained by microbial N, P} \]

\[ R_{h} \text{ constrained by substrate DOC, } T_{c} \text{ and } \psi \]

\[ R_{h} \text{ constrained by O}_{2} \]

\[ \psi_{h} \text{ constraints on microbial growth} \]

O\text{2 demand driven by potential } R_{h} \]

active uptake coupled with radial diffusion of O\text{2} \]

maintenance respiration

temperature sensitivity of } R_{m} \]

growth respiration

DOC uptake driven by } R_{g} \]  

[A7a]

[A7b]

[A7c]

[A8]

[A9]

[A10]

[A11]

[A12]

[A13]

[A14]

[A15]

[A16]

[A17a]

[A17b]

[A18]

[A19]

[A20]

[A21]
DON, DOP uptake driven by $U_{\text{on}, \text{IC}}$ [A22]

first-order decay of microbial C, [A23]
decay of microbial N, P [A24]

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

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

**Microbial Nutrient Exchange**

\[ U_{\text{NH}_4 n, j, l} = (M_{\text{n}, n, j, l, C} C_{\text{Nj}} - M_{\text{n}, n, j, l, N}) \]

\[ U_{\text{NH}_4 l, n, j, l} = \min \left\{ (M_{\text{n}, n, j, l, C} C_{\text{Nj}} - M_{\text{n}, n, j, l, N}), \frac{U'_{\text{NH}_4}}{a_{\text{n}, n, j, l}} \left( [\text{NH}_4^+_{\text{n}, n, j, l}] - [\text{NH}_4^+_{\text{nm}}] \right) / \left( [\text{NH}_4^+_{\text{n}, n, j, l}] - [\text{NH}_4^+_{\text{nm}}] + K_{\text{NH}_4} \right) \right\} \]

\[ U_{\text{NO}_3 n, j, l} = \min \left\{ (M_{\text{n}, n, j, l, C} C_{\text{Nj}} - (M_{\text{n}, n, j, l, N} + U_{\text{NH}_4 n, j, l})), \frac{U'_{\text{NO}_3}}{a_{\text{n}, n, j, l}} \left( [\text{NO}_3^-_{\text{n}, n, j, l}] - [\text{NO}_3^-_{\text{nm}}] \right) / \left( [\text{NO}_3^-_{\text{n}, n, j, l}] - [\text{NO}_3^-_{\text{nm}}] + K_{\text{NO}_3} \right) \right\} \]

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

\[ U_{\text{PO}_4 n, j, l} = \min \left\{ (M_{\text{n}, n, j, l, C} C_{\text{Pj}} - M_{\text{n}, n, j, l, P}), \frac{U'_{\text{PO}_4}}{a_{\text{n}, n, j, l}} \left( [\text{H}_2\text{PO}_4^-_{\text{n}, n, j, l}] - [\text{H}_2\text{PO}_4^-_{\text{nm}}] \right) / \left( [\text{H}_2\text{PO}_4^-_{\text{n}, n, j, l}] - [\text{H}_2\text{PO}_4^-_{\text{nm}}] + K_{\text{PO}_4} \right) \right\} \]

\[ \phi_{\text{P}, n, f, j, l} = \max \{ 0, M_{\text{n}, n, f, j, l, C} C_{\text{Nj}} - M_{\text{n}, n, f, j, l, N} - \max \{ 0, U_{\text{on}, n, f, j, l} \} \} \]

\[ R_{\phi, n, f, j, l} = E_\phi \phi_{\text{P}, n, f, j, l} \]

\[ \delta M_{\text{n}, n, j, L N} / \delta t = F_j U_{\text{n}, n, L N} + U_{\text{NH}_4 n, j, l} + U_{\text{NO}_3 n, j, l} + \phi_{\text{P}, n, f, j, l} - D_{\text{m}, n, j, L N} \]

\[ \delta M_{\text{n}, n, j, L P} / \delta t = F_j U_{\text{n}, n, L P} + U_{\text{PO}_4 n, j, l} - D_{\text{m}, n, j, L P} \]

\[ M_{\text{n}, n, j, L C} = M_{\text{n}, n, j, \text{labile}, l, C} + M_{\text{n}, n, j, \text{resistant}, l, C} F_t / F_1 \]
Humification

decomposition products of litter substrate added to POC depending on lignin

\[ H_{Si,lignin,l,C} = D_{Si,lignin,l,C} \]

\[ H_{Si,lignin,l,N,P} = D_{Si,lignin,l,N,P} \]

\[ H_{Si,lignin,l,C} = H_{Si,lignin,l,C} L_{hj} \]

\[ H_{Si,lignin,l,N,P} = H_{Si,lignin,l,C} S_{l,l,N,P} / S_{l,l,C} \]

\[ H_{Mi,n,j,l,C} = D_{Mi,n,j,l,C} F_{h} \]

\[ H_{Mi,n,j,l,N,P} = H_{Mi,n,j,l,C} M_{l,n,j,l,N,P} / M_{l,n,j,l,C} \]

\[ F_{h} = 0.167 + 0.167 F_{clay} + 0.167 \times 10^{-6} G_{l,l,C} \]

\[ H_{Zi,n,j,l,C} = D_{Mi,n,j,l,C} - H_{Mi,n,j,l,C} \]

\[ H_{Zi,n,j,l,N,P} = D_{Mi,n,j,l,N,P} - H_{Mi,n,j,l,N,P} \]
**Definition of Variables in Section A**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Equation</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>subscripts</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>i</td>
<td>substrate-microbe complex: coarse woody litter, fine non-woody litter, POC, humus</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>j</td>
<td>kinetic component: labile l, resistant r, active a</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>l</td>
<td>soil or litter layer</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>n</td>
<td>microbial functional type: heterotrophic (bacteria, fungi), autotrophic (nitrifiers, methanotrophs), diazotrophic, obligate aerobe, facultative anaerobes (denitrifiers), obligate anaerobes (methanogens)</td>
<td></td>
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</tr>
<tr>
<td><strong>variables</strong></td>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>$A_i,l,c$</td>
<td>mass of adsorbed SOC</td>
<td>g C m$^{-2}$</td>
<td>[A1c,A2c]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$[A_i,l,c]$</td>
<td>concentration of adsorbed SOC in soil</td>
<td>g C Mg$^{-1}$</td>
<td>[A4c]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$a$</td>
<td>microbial surface area</td>
<td>m$^2$ m$^{-2}$</td>
<td>[A26]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$B$</td>
<td>parameter such that $f_{tg} = 1.0$ at $T_l = 298.15$ K</td>
<td></td>
<td>[A6]</td>
<td>26.235</td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>Freundlich exponent for sorption isotherm</td>
<td></td>
<td>[A8]</td>
<td>0.85</td>
<td>Grant et al. (1993a,b)</td>
</tr>
<tr>
<td>$\beta$</td>
<td>specific colonization rate of uncolonized substrate</td>
<td>-</td>
<td>[A5]</td>
<td>2.5</td>
<td>Grant et al. (2010)</td>
</tr>
<tr>
<td>$C_{N,P,n,a,l}$</td>
<td>ratio of $M_{i,r,a,N,P}$ to $M_{i,r,a,C}$</td>
<td>g N or P g C$^{-1}$</td>
<td>[A12]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
<td>Value</td>
<td>Source</td>
<td></td>
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<tr>
<td>-----------------</td>
<td>-----------------------------------------------------------------------------</td>
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</tr>
<tr>
<td>$C_{N,P}$</td>
<td>maximum ratio of $M_{i,n,l,j,N,P}$ to $M_{i,n,l,j,C}$ maintained by $M_{i,n,l,j,C}$</td>
<td>g N or P g C$^{-1}$</td>
<td>0.22 and 0.13 (N), 0.022 and 0.013 (P) for $j =$ labile and resistant, respectively</td>
<td>Grant et al. (1993a,b)</td>
<td></td>
</tr>
<tr>
<td>$D_{A_i,j,C}$</td>
<td>decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ producing $Q$ in [A13]</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A1c,A7c,A31c]</td>
<td>Grant et al. (1993a,b)</td>
<td></td>
</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>specific decomposition rate of $A_{i,l,C}$ by $M_{i,d,l,C}$ at 25°C and saturating[A$_{i,l,C}$]</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A4c]</td>
<td>0.025</td>
<td>Grant et al. (1993a,b)</td>
</tr>
<tr>
<td>$D_{M_{i,n,j,l,N,P}}$</td>
<td>decomposition rate of $A_{i,n,j,l,N,P}$ by $M_{i,d,l,C}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A24,A29,A39]</td>
<td></td>
<td>Grant et al. (1993a,b)</td>
</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A1a,A4c]</td>
<td>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</td>
<td>Grant et al. (1993a,b)</td>
</tr>
<tr>
<td>$D_{M_{i,n,j,l,N,P}}$</td>
<td>decomposition rate of $M_{i,n,j,l,N,P}$ by $M_{i,d,l,C}$</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A23,A25,A35,A38]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating $[S_{i,j,C}]$</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A1a,A7a,A31a]</td>
<td></td>
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</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>specific decomposition rate of $M_{i,n,j,l}$ at 30°C</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A23,A24]</td>
<td></td>
<td>Grant et al. (1993a,b)</td>
</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>decomposition rate of $M_{i,n,l,j,C}$</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A23,A25,A35,A38]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{A_i,l,C}$</td>
<td>decomposition rate of $M_{i,n,j,l,N,P}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A24,A29,A39]</td>
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<tr>
<td>$D_{S_{i,j,l,C}}$</td>
<td>decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing $Q$ in [A13]</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A1a,A7a,A31a]</td>
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<tr>
<td>$D_{S_{i,j,C}}$</td>
<td>specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating $[S_{i,j,C}]$</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A4a]</td>
<td></td>
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<tr>
<td>$D_{S_{i,j,l,N,P}}$</td>
<td>decomposition rate of $S_{i,j,l,N,P}$ by $\Sigma_n M_{i,n,a,l}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A7a, A32]</td>
<td></td>
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<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
<td>Reference</td>
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<tr>
<td>$D'_{Si,j,l,C}$</td>
<td>specific decomposition rate of $S_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A1a,A4a]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{O_2,l}$</td>
<td>aqueous dispersivity–diffusivity of O$_2$ during microbial uptake in soil</td>
<td>m$^2$ h$^{-1}$</td>
<td>[A17]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$D_{Zi,j,l,C}$</td>
<td>decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ producing $Q$ in [A13]</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A1b,A7b]</td>
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<tr>
<td>$D_{Zi,j,N,P}$</td>
<td>decomposition rate of $Z_{i,j,N,P}$ by $\Sigma_n M_{i,n,a,l}$</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A7b]</td>
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<tr>
<td>$D_{Zi,C}$</td>
<td>specific decomposition rate of $Z_{i,j,l,C}$ by $\Sigma_n M_{i,n,a,l}$ at 25°C and saturating[Z$_{i,l,C}$]</td>
<td>g C g C$^{-1}$ h$^{-1}$</td>
<td>[A4b]</td>
<td></td>
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</tr>
<tr>
<td>$\Delta G_x$</td>
<td>energy yield of C oxidation with different reductants $x$</td>
<td>kJ g C$^{-1}$</td>
<td>[A21] 37.5 ($x = O_2$), 4.43 ($x = DOC$)</td>
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<tr>
<td>$E_m$</td>
<td>energy requirement for growth of $M_{i,n,a,l}$</td>
<td>kJ g C$^{-1}$</td>
<td>[A21] 25</td>
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<tr>
<td>$E_\Phi$</td>
<td>energy requirement for non-symbiotic N$_2$ fixation by heterotrophic diazotrophs ($n = f$)</td>
<td>g C g N$^{-1}$</td>
<td>[A28] 5</td>
<td></td>
<td></td>
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<tr>
<td>$F_{clay}$</td>
<td>fraction of mineral soil as clay</td>
<td>Mg Mg$^{-1}$</td>
<td>[A37]</td>
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<td></td>
</tr>
<tr>
<td>$F_h$</td>
<td>fraction of products from microbial decomposition that are humified (function of clay content)</td>
<td></td>
<td>[A35, A37] Sørenson (1981)</td>
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<tr>
<td>$F_1$</td>
<td>fraction of microbial growth allocated to labile component $M_{i,n,l}$</td>
<td></td>
<td>[A25,A29,A30] 0.55 Grant et al. (1993a,b)</td>
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<tr>
<td>$F_r$</td>
<td>fraction of microbial growth allocated to resistant component $M_{i,n,r}$</td>
<td></td>
<td>[A25,A29,A30] 0.45 Grant et al. (1993a,b)</td>
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<tr>
<td>$F_s$</td>
<td>equilibrium ratio between $Q_{i,l,C}$ and $H_{i,l,C}$</td>
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<td>[A8]</td>
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<td>$f_{dl,n,N,P}$</td>
<td>fraction of N or P released with $D_{Ml,n,j,l,C}$ during decomposition</td>
<td>dimensionless</td>
<td>[A24] 0.33 $U_{NH_4} &gt; 0$ 1.00 $U_{NH_4} &lt; 0$ 0.33 $U_{PO_4} &gt; 0$ 1.00 $U_{PO_4} &lt; 0$</td>
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<td>$f_{tg_l}$</td>
<td>temperature function for microbial growth respiration</td>
<td>dimensionless</td>
<td>[A1,A6,A13]</td>
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<td>Description</td>
<td>Unit</td>
<td>Source</td>
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<tr>
<td>$f_{ml}$</td>
<td>temperature function for maintenance respiration</td>
<td>dimensionless</td>
<td>[A18,A19]</td>
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<tr>
<td>$f_{vgl}$</td>
<td>soil water potential function for microbial, root or mycorrhizal growth respiration</td>
<td>dimensionless</td>
<td>[A13,A15]</td>
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<tr>
<td>$\phi_{l,n=f,j,l}$</td>
<td>non-symbiotic N$_2$ fixation by heterotrophic diazotrophs ($n=f$)</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A27,A28,A29]</td>
<td></td>
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<tr>
<td>$G_{l,IC}$</td>
<td>total C in substrate-microbe complex</td>
<td>g C Mg$^{-1}$</td>
<td>[A1,A2c,A3a,A8,A37]</td>
<td></td>
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<tr>
<td>$[H_2PO_4^-]$</td>
<td>concentration of H$_2$PO$_4^-$ in soil solution</td>
<td>g P m$^{-3}$</td>
<td>[A26]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$H_a$</td>
<td>energy of activation</td>
<td>J mol$^{-1}$</td>
<td>[A6,C10] 65 x 10$^3$</td>
<td>Addiscott (1983)</td>
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<tr>
<td>$H_{da}$</td>
<td>energy of high temperature deactivation</td>
<td>J mol$^{-1}$</td>
<td>[A6,C10] 225 x 10$^3$</td>
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<tr>
<td>$H_{dl}$</td>
<td>energy of low temperature deactivation</td>
<td>J mol$^{-1}$</td>
<td>[A6,C10] 195 x 10$^3$</td>
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<tr>
<td>$H_{Mn,n,j,l,IC}$</td>
<td>transfer of microbial C decomposition products to humus</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A35,A36,A38]</td>
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<tr>
<td>$H_{Mn,n,j,l,N,P}$</td>
<td>transfer of microbial N or P decomposition products to humus</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A36,A39]</td>
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<tr>
<td>$H_{Si,j,l,IC}$</td>
<td>transfer of C hydrolysis products to particulate OM</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A31,A32,A33,A34]</td>
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<tr>
<td>$H_{Si,j,l,N,P}$</td>
<td>transfer of N or P hydrolysis products to particulate OM</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A32,A34]</td>
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<tr>
<td>$H_{Zi,n,j,l,IC}$</td>
<td>transfer of microbial C decomposition products to microbial residue</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A38]</td>
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<tr>
<td>$H_{Zi,n,j,l,N,P}$</td>
<td>transfer of microbial N or P decomposition products to microbial residue</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A39]</td>
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<tr>
<td>$K_{IS}$</td>
<td>inhibition constant for microbial colonization of substrate</td>
<td>-</td>
<td>[A5] 0.5</td>
<td>Grant et al. (2010)</td>
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<tr>
<td>$K_{NH_4}$</td>
<td>M-M constant for NH$_4^+$ uptake at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td>[A26] 0.40</td>
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<tr>
<td>$K_{NO_3}$</td>
<td>M-M constant for NO$_3^-$ uptake at microbial surfaces</td>
<td>g N m$^{-3}$</td>
<td>[A26] 0.35</td>
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<tr>
<td>$K_{PO_4}$</td>
<td>M-M constant for H$_2$PO$_4^-$ uptake at microbial surfaces</td>
<td>g P m$^{-3}$</td>
<td>[A26] 0.125</td>
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<tr>
<td>$K_{ID}$</td>
<td>inhibition constant for $[M_{i,n,a}]$ on $S_{i,C},Z_{i,C}$</td>
<td>g C m$^{-3}$</td>
<td>[A4] 25</td>
<td>Grant et al.</td>
<td></td>
</tr>
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</table>
$K_mD$ Michaelis–Menten constant for $D_{i,j,C}$ g C Mg$^{-1}$ [A4] 75 (1993a,b); Lizama and Suzuki (1990)

$K_mQ_C$ Michaelis–Menten constant for $R'_{i,b,n}$ on $Q_{i,C}$ g C m$^{-3}$ [A13] 36 Griffin (1972)

$K_{O_2}$ Michaelis–Menten constant for reduction of $O_2$ by microbes, roots and mycorrhizae g O$_2$ m$^{-3}$ [A17] 0.32 Grant et al. (1993a,b)

$k_{ts}$ equilibrium rate constant for sorption h$^{-1}$ [A8] 0.01 Shulten and Schnitzer (1997)

$L_{hi}$ 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

$M$ molecular mass of water g mol$^{-1}$ [A15]

$M_{i,a,n,C}$ heterotrophic microbial C used for decomposition g C m$^{-2}$ [A1,A3a,A4]

$M_{i,a,j,n,C}$ microbial C g C m$^{-2}$ [A13,A17A23,A25,A26, A30,A36]

$M_{i,a,j,N}$ microbial N g N m$^{-2}$ [A18,A27,A29]

$M_{i,a,j,P}$ microbial P g P m$^{-2}$ [A24,A29,A26, A36]

$M_{i,a,a,l,C}$ active microbial C from heterotrophic population $n$ associated with $G_{i,l,C}$ g C m$^{-2}$ [A3,A13,A17, A30]

$[M_{i,a,a,l,C}]$ concentration of $M_{i,a,a,l,C}$ in soil water = $M_{i,a,a,l,C}/\theta_l$ g C m$^{-3}$ [A3, A5]

$n$ number of microbial microsites m$^{-2}$ [A17b]

$[\text{NH}_4^+,i,n,j,l]$ concentration of $\text{NH}_4^+$ at microbial surfaces g N m$^{-3}$ [A26]

$[\text{NH}_4^+,\text{ma}]$ concentration of $\text{NH}_4^+$ at microbial surfaces below which $U_{\text{NH}_4} = 0$ g N m$^{-3}$ [A26] 0.0125

$[\text{NO}_3^-,i,n,j,l]$ concentration of $\text{NO}_3^-$ at microbial surfaces g N m$^{-3}$ [A26]
**[NO₃⁻]_{mn}** concentration of NO₃⁻ at microbial surfaces below which \( U_{NO₃} = 0 \)
g N m⁻³ \[A26\] 0.03

**[H₂PO₄⁻]_{i,n,j,l}** concentration of H₂PO₄⁻ at microbial surfaces
g N m⁻³ \[A26\]

**[H₂PO₄⁻]_{mn}** concentration of H₂PO₄⁻ at microbial surfaces below which \( U_{PO₄} = 0 \)
g N m⁻³ \[A26\] 0.002

**[O₂]_{2m,a,l}** O₂ concentration at heterotrophic microsites
g O₂ m⁻³ \[A17\]

**[O₂]_{2a}** O₂ concentration in soil solution
g O₂ m⁻³ \[A17\]

**[Q]_{i,l,C}** DOC from products of \( D_{Si,j,l,C} \) [A3] and \( D_{Zi,j,l,C} \) [A5]
g C m⁻² \[A8,A13,A22\]

**[Q]_{i,l,C}** solution concentration of \( Q_{i,l,C} \)
g C Mg⁻¹ \[A8,A13\]

**[Q]_{i,l,N}** DON and DOP from products of \( (D_{Si,j,l,N,P} + D_{Zi,j,l,N,P}) \)
g N or P m⁻² \[A9,A22\]

**q_m** rate constant for reallocating \( M_{i,a,l,C} \) to \( M_{i,d,l,C} \)
h⁻¹ \[A3a\] 0.5

**R** gas constant
J mol⁻¹ K⁻¹ \[A6,A15,C10\] 8.3143

**R_{φ,n=f,j,l}** respiration for non-symbiotic N₂ fixation by heterotrophic diazotrophs (\( n = f \))
g C m⁻² h⁻¹ \[A28\]

**R_{g,j,n,l}** growth respiration of \( M_{i,p,a,l} \) on \( Q_{i,l,C} \) under nonlimiting O₂ and nutrients

g C g C⁻¹ h⁻¹ \[A20\]

**R_h** total heterotrophic respiration of all \( M_{i,p,a,l} \) under ambient DOC, O₂, nutrients, \( θ \) and temperature

g C m⁻² h⁻¹ \[A11\]

**R_{h,n,a,l}** heterotrophic respiration of \( M_{i,n,a,l} \) under ambient DOC, O₂, nutrients, \( θ \) and temperature

g C m⁻² h⁻¹ \[A5,A11,A14,A20 \]

**R_{h,n,l}** specific heterotrophic respiration of \( M_{i,n,a,l} \) under nonlimiting O₂, DOC, \( θ \) and 25°C

g C g C⁻¹ h⁻¹ \[A12,A13\]

**R_{h,a}** specific heterotrophic respiration of \( M_{i,n,a,l} \) under nonlimiting DOC, O₂, nutrients, \( θ \) and 25°C

g C g C⁻¹ h⁻¹ \[A12\] 0.125 Shields et al. (1973)

**R_{h,a}’** heterotrophic respiration of \( M_{i,n,a,l} \) under nonlimiting O₂ and ambient DOC, nutrients, \( θ \) and temperature

g C m⁻² h⁻¹ \[A13,A14,A16\]

**R_m** specific maintenance respiration at 25°C

g C g N⁻¹ h⁻¹ \[A18\] 0.0115 Barnes et al. (1998)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Reference(s)</th>
<th>Notes</th>
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<td>$R_{m,n,j,l}$</td>
<td>maintenance respiration by $M_{i,n,j,l}$</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A18, A20, A21, A25]</td>
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<tr>
<td>$\sigma$</td>
<td>shape parameter in $f_{\psi g}$</td>
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<td>[A15]</td>
<td>0.2</td>
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<tr>
<td>$r_{wl}$</td>
<td>radius of $r_m$ + water film at current water content</td>
<td>m</td>
<td>[A17]</td>
<td></td>
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<tr>
<td>$r_m$</td>
<td>radius of heterotrophic microsite</td>
<td>m</td>
<td>[A17]</td>
<td>2.5 x 10$^{-6}$</td>
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<tr>
<td>$r_{wl}$</td>
<td>thickness of water films</td>
<td>m</td>
<td>[A17]</td>
<td></td>
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<tr>
<td>$S$</td>
<td>change in entropy</td>
<td>J mol$^{-1}$ K$^{-1}$</td>
<td>[A6, C10]</td>
<td>710</td>
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<tr>
<td>$[S_{i,j,l,c}]$</td>
<td>concentration of $S_{i,j,l,c}$ in soil</td>
<td>g C Mg$^{-1}$</td>
<td>[A4a]</td>
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<tr>
<td>$S_{i,j,l,c}$</td>
<td>mass of colonized litter, POC or humus C</td>
<td>g C m$^{-2}$</td>
<td>[A2a, A5, A7a, A33]</td>
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<tr>
<td>$S'_{i,j,l,c}$</td>
<td>mass of uncolonized litter, POC or humus C</td>
<td>g C m$^{-2}$</td>
<td>[A5]</td>
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<tr>
<td>$S_{i,j,l,N,P}$</td>
<td>mass of litter, POC or humus N or P</td>
<td>g N or P m$^{-2}$</td>
<td>[A7a, A33]</td>
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<tr>
<td>$T_d$</td>
<td>soil temperature</td>
<td>K</td>
<td>[A6, A15, A19]</td>
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<tr>
<td>$U_{i,n,c}$</td>
<td>uptake of $Q_{i,c}$ by $\Sigma_{n}M_{i,n,a,l}$ under limiting nutrient availability</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A5, A21, A22, A25]</td>
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<tr>
<td>$U_{i,n,N,P}$</td>
<td>uptake of $Q_{i,N,P}$ by $\Sigma_{n}M_{i,n,a,l}$ under limiting nutrient availability</td>
<td>g N or P m$^{-2}$ h$^{-1}$</td>
<td>[A22, A29]</td>
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<tr>
<td>$U_{NH4,i,n,j,l}$</td>
<td>NH$_4^+$ uptake by microbes</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26, A27, A29]</td>
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<tr>
<td>$U'_{NH4}$</td>
<td>maximum $U_{NH4}$ at 25 °C and non-limiting NH$_4^+$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26]</td>
<td>5.0 x 10$^{-3}$</td>
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<tr>
<td>$U_{NO3,i,n,j,l}$</td>
<td>NO$_3^-$ uptake by microbes</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26, A27, A29]</td>
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<tr>
<td>$U'_{NO3}$</td>
<td>maximum $U_{NO3}$ at 25 °C and non-limiting NO$_3^-$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26]</td>
<td>5.0 x 10$^{-3}$</td>
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<td>$U_{O2,i,n}$</td>
<td>O$<em>2$ uptake by $M</em>{i,n,a,l}$ under ambient O$_2$</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[A14, A17]</td>
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### Symbols and Units

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<td>$U'_{O_2,i}$</td>
<td>O$<em>2$ uptake by $M</em>{i,j,k,l}$ under nonlimiting O$_2$</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[A14,A16,A17]</td>
</tr>
<tr>
<td>$U'_{PO_4,i,j,k,l}$</td>
<td>H$_2$PO$_4^-$ uptake by microbes</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26,A27,A29]</td>
</tr>
<tr>
<td>$U'_{PO_4}$</td>
<td>maximum $U_{PO_4}$ at 25 °C and non-limiting H$_2$PO$_4^-$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[A26] 5.0 x 10$^{-3}$</td>
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<td>$X_{i,j,C}$</td>
<td>adsorbed C hydrolysis products</td>
<td>g C Mg$^{-1}$</td>
<td>[A8,A10]</td>
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<tr>
<td>$X_{i,j,N,P}$</td>
<td>adsorbed N or P hydrolysis products</td>
<td>g P Mg$^{-1}$</td>
<td>[A10]</td>
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<td>$y$</td>
<td>selected to give a $Q_{10}$ for $f_{im}$ of 2.25</td>
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<td>[A19] 0.081</td>
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<td>$\psi_s$</td>
<td>soil or residue water potential</td>
<td>MPa</td>
<td>[A15]</td>
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<tr>
<td>$Y_{i,j,C}$</td>
<td>sorption of C hydrolysis products</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[A8,A9,A10]</td>
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<tr>
<td>$Y_{i,j,N,P}$</td>
<td>sorption of N or P hydrolysis products</td>
<td>g P m$^{-2}$ h$^{-1}$</td>
<td>[A9,A10]</td>
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<tr>
<td>$[Z_{i,j,C}]$</td>
<td>concentration of $Z_{i,j,C}$ in soil</td>
<td>g C Mg$^{-1}$</td>
<td>[A4b]</td>
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<tr>
<td>$Z_{i,j,C}$</td>
<td>mass of microbial residue C in soil</td>
<td>g C m$^{-2}$</td>
<td>[A2b,A7b]</td>
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<tr>
<td>$Z_{i,j,N,P}$</td>
<td>mass of microbial residue N or P in soil</td>
<td>g P m$^{-2}$</td>
<td>[A7b]</td>
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Section C: Gross Primary Productivity, Autotrophic Respiration, Growth and Litterfall

\[ GPP = \sum_{i,j,k,l,m,n,o} (V_{ci,j,k,l,m,n,o} = V_{gi,j,k,l,m,n,o}) A_{i,j,k,l,m,n,o} \]

\[ V_{gi,j,k,l,m,n,o} = (C_b - C_{ui,j,k,l,m,n,o}) / r_{ui,j,k,l,m,n,o} \]

\[ V_{ci,j,k,l,m,n,o} = \min \{V_{bi,j,k,l,m,n,o}, V_{ji,j,k,l,m,n,o} \} \]

\[ r_{ui,j,k,l,m,n,o} = r_{mini,j,k,l,m,n,o} + (r_{maxi} - r_{mini,j,k,l,m,n,o}) e(\beta \psi_i) \]

\[ r_{mini,j,k,l,m,n,o} = (C_b - C_{ci,j,k,l,m,n,o}) / V_{ci,j,k,l,m,n,o} \]

\[ V_{bi,j,k,l,m,n,o} = V_{bmax,j,k} (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (C_{ci,j,k,l,m,n,o} + K_{c_i}) f_V i,j,k,l,m,n,o \]

\[ V_{bmax,i,j,k} = V_{bmax}' F_{rubisco} M_{i,j,k,prot} / A_{i,j,k} f_{int} f_i \]

\[ \Gamma_{i,j,k} = 0.5 O_{c} V_{omax,i,j,k} K_{c_i} / (V_{omax,i,j,k} K_o) \]

\[ V_{omax,i,j,k} = V_{o}' F_{rubisco} M_{i,j,k,prot} / A_{i,j,k} f_{o} \]

\[ K_{c_i} = K_{c_i} f_{kcl} (1 + O_{c} / (K_o f_{kcl})) \]

\[ V_{ji,j,k,l,m,n,o} = J_{i,j,k,l,m,n,o} Y_{i,j,k,l,m,n,o,f} i,j,k,l,m,n,o \]

\[ Y_{i,j,k,l,m,n,o} = (C_{ci,j,k,l,m,n,o} - \Gamma_{i,j,k}) / (4.5 C_{ci,j,k,l,m,n,o} + 10.5 \Gamma_{i,j,k}) \]

\[ J_{i,j,k,l,m,n,o} = (J_{i,j,k,l,m,n,o} f_{maxy} - J_{i,j,k,l,m,n,o} f_{maxy})^2 - 4 \alpha e_{i,l,m,n,o} J_{i,j,k,l,m,n,o} f_{maxy} \]

\[ J_{maxy,j,k} = V_{j}' F_{chlorophyll} M_{i,j,k,prot} / A_{i,j,k} f_{j} f_{c} \]

\[ f_V i,j,k,l,m,n,o = (r_{mini,j,k,l,m,n,o} / r_{i,j,k,l,m,n,o})^{0.5} \]
\[ f_{tot} = \exp[B_o - H_{o2}/(RT_{c0})] / [1 + \exp[(H_{at} - ST_{c0}) / (RT_{c0})] + \exp((ST_{c0} - H_{at}) / (RT_{c0}))] \]

\[ f_{tot} = \exp[B_o - H_{o2}/(RT_{c0})] / [1 + \exp[(H_{at} - ST_{c0}) / (RT_{c0})] + \exp((ST_{c0} - H_{at}) / (RT_{c0}))] \]

\[ f_{i} = \exp[B_i - H_{i2}/(RT_{c0})] / [1 + \exp[(H_{at} - ST_{c0}) / (RT_{c0})] + \exp((ST_{c0} - H_{at}) / (RT_{c0}))] \]

\[ f_{kci} = \exp[B_{k-c} - H_{k-c}/(RT_{c0})] \]

\[ f_{kci} = \exp[B_{k-c} - H_{k-c}/(RT_{c0})] \]

\[ f_{Ci} = \min(\sigma_{N_i} / (\sigma_{N_c} + \sigma_{C_{i,c}}/K_{C_{i,c}}), \sigma_{P_{ij}} / (\sigma_{P_{ij}} + \sigma_{C_{i,c}}/K_{C_{i,c}})) \]

\[ \delta M_{R_{i,j,k}} / \delta t = \delta M_{1_{i,j,k}} / \delta t \min\left[\left[N_{\text{leaf}} + (N_{\text{leaf}} - N_{\text{leaf}}) f_{Ci}\right] / N_{\text{prot}}, \left[P'_{\text{leaf}} + (P_{\text{leaf}} - P_{\text{leaf}}) f_{Ci}\right] / P_{\text{prot}}\right] \]

**Autotrophic Respiration**

\[ R_a = \Sigma_i \Sigma_j (R_{c1} + R_{at}) + \Sigma_i \Sigma_j (R_{c1r,l} + R_{atr,l}) + E_{\text{N,P}} (U_{\text{NH4},r,l} + U_{\text{NO3},r,l} + U_{\text{PO4},r,l}) \]

\[ R_{c1} = R_c \sigma_{C_{i,j,l}} f_{\text{uai}} \]

\[ R_{c1r,l} = R_c \sigma_{C_{i,r,l}} f_{\text{uai},l} (U_{O2r,l} / U'_{O2r,l}) \]

\[ U_{O2r,l} = U'_{O2r,l} \left[[O_{2l,r}]/([O_{2l,r}] + K_{O2})\right] \]

\[ = U_{u_{l,r},l}[O_{2l}] + 2\pi L_{r,r,l} D_{O2} ([O_{2l}] - [O_{2l,r,l}]) \ln((r_{at} + r_{at,l}) / r_{at,l}) + 2\pi L_{r,r,l} D_{O2} ([O_{2l,r,l}] - [O_{2l,r,l}]) \ln((r_{at} + r_{at,l}) / r_{at,l}) \]

\[ U'_{O2r,l} = 2.67 R_c'_{l,r,l} \]

Arhenius functions for carboxylation, oxygenation and electron transport temperature sensitivity of \( K_{c}, K_{o} \)

control of \( \sigma_{N_i} \) and \( \sigma_{P_{ij}} \) vs. \( \sigma_{C_{i,c}} \) in shoots on \( V_{at} \), \( V_j \) through product inhibition and on leaf protein growth through leaf structural C:N:P ratios growth of remobilizable leaf protein C

total autotrophic respiration

O\(_3\) 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

[C10a] [C10b] [C10c] [C10d] [C10e] [C11] [C12] [C13] [C14a] [C14b] [C14c] [C14d] [C14e]
\[ R_{ai,j} = \min\{0.0, R_{ci,j} - R_{mi,j}\} \]

\[ R_{ai,r,l} = \min\{0.0, R_{ci,r,l} - R_{mi,r,l}\} \]

\[ R_{mi,j} = \sum_{z} (N_{ij,z} R_{m'} f_{m'+}) \]

\[ R_{mi,r,l} = \sum_{z} (N_{ir,l,z} R_{m'} f_{m'+}) \]

\[ R_{gi,j} = \max\{0.0, \min\{(R_{ci,j} - R_{mi,j}) \min\{1.0, \max\{0.0, \psi_{i} - \psi'_{i}\}\}\}\} \]

\[ R_{gi,r,l} = \max\{0.0, \min\{(R_{ci,r,l} - R_{mi,r,l}) \min\{1.0, \max\{0.0, \psi_{i,l} - \psi'_{i,l}\}\}\}\} \]

**Growth and Litterfall**

\[ l_{ij,\text{C}} = R_{ai,j} M_{i,j} / M_{g(i,j)} \]

\[ l_{ij,\text{N}} = l_{ij,\text{C}} N_{\text{prot}} (1.0 - X_{\text{mix}} f_{i,j,N(i,j)}) \]

\[ l_{ij,\text{P}} = l_{ij,\text{C}} P_{\text{prot}} (1.0 - X_{\text{mix}} f_{i,j,P(i,j)}) \]

\[ f_{i,j,N} = \sigma_{C_{i,j}} / (\sigma_{C_{i,j}} + \sigma_{N_{i,j}}/K_{\text{SN}}) \]

\[ f_{i,j,P} = \sigma_{C_{i,j}} / (\sigma_{C_{i,j}} + \sigma_{P_{i,j}}/K_{\text{SP}}) \]

\[ x_{i,r,l,C} = r_{x} \sigma_{C_{i,r,l}} \]

\[ x_{i,r,l,N} = r_{x} \sigma_{N_{i,r,l}} f_{i,r,l,N} \]

\[ x_{i,r,l,P} = r_{x} \sigma_{P_{i,r,l}} f_{i,r,l,P} \]

\[ f_{i,r,l,N} = \sigma_{N_{i,j}} / (\sigma_{N_{i,j}} + \sigma_{C_{i,j}}/K_{\text{SN}}) \]

\[ f_{i,r,l,P} = \sigma_{P_{i,j}} / (\sigma_{P_{i,j}} + \sigma_{C_{i,j}}/K_{\text{SP}}) \]

remobilization in branches, roots and mycorrhizae when \( R_m > R_c \) \[ \text{[C15]} \]

maintenance respiration of branches, roots and mycorrhizae \[ \text{[C16]} \]

growth respiration of branches, roots and mycorrhizae when \( R_m < R_c \) \[ \text{[C17]} \]

senescence drives litterfall of non-remobilizable material \[ \text{[C18]} \]

litterfall of N and P is driven by that of C but reduced by translocation of remobilizable N and P to \( \sigma_{N} \) and \( \sigma_{P} \) according to ratios of \( \sigma_{N} \) and \( \sigma_{P} \) with \( \sigma_{C} \). root and mycorrhizal litterfall \((i,r,l)\) is calculated as for branch litterfall \((i,j,z)\) \[ \text{[C19a]} \]

root and mycorrhizal exudation driven by \( \sigma_{C} \), \( \sigma_{N} \) and \( \sigma_{P} \), and by \( \sigma_{C} : \sigma_{N} \) and \( \sigma_{C} : \sigma_{P} \) \[ \text{[C19b, C19c]} \]

\[ \text{[C19d]} \]

\[ \text{[C19e]} \]

\[ \text{[C19f]} \]

\[ \text{[C19g]} \]

\[ \text{[C19h]} \]

\[ \text{[C19i]} \]
\( \delta M_{Bij}/\delta t = \Sigma [R_{Gij}(1 - Y_{Gij}) / Y_{Gij}] - R_{Bij} - l_{ij,c} \)

\( \delta M_{Rir,t}/\delta t = [R_{Gir}(1 - Y_{Gir}) / Y_{Gir}] - R_{Rir,t} - l_{r,t,c} \)

\( \delta A_{ij,k,t}/\delta t = \chi (M_{ij,k,t}/y) ^{0.33} \delta M_{ij,k,t}/\delta t \min \{1, \max \{0, y_G - y'_G\} \}

\( \delta L_{r,t,l}/\delta t = (\delta M_{Rir,t,l}/\delta t) / y_i \nu_r / (p_r (1 - \theta p_r) (\pi r_{r,t,l})^2) \)

\( \delta L_{r,t,l,2}/\delta t = (\delta M_{Rir,t,l}/\delta t) / y_i \nu_r / (p_r (1 - \theta p_r) (\pi r_{r,t,l})^2) \)

\( f_{\text{init}} = T_i \{ \exp \{ B_c - H_{av} / (RT_c) \} \} / \{1 + \exp \{ (H_{av} - ST_{ci}) / (RT_{ci}) \} + \exp \{ (ST_{ci} - H_{av}) / (RT_{ci}) \} \}

\( f_{\text{init}} = e^{0.0811 (T_i / 298.15)} \)

### Root and Mycorrhizal Nutrient Uptake

\[ U_{NH4,t} = \{ U_{wir} [NH_4^+] + 2\pi L_{r,t} D_{NH4} ([NH_4^+] - [NH_4^+]) / \ln(d_{r,t} / r_{r,t,c}) \} \]

\[ = U'_{NH4}(U_{O2r,t} / U'_{O2r,t}) A_{r,t} ([NH_4^+] - [NH_4^+]) / ([NH_4^+] - [NH_4^+]) + K_{NH4} f_{\text{init}} f_{\text{init},r,t} \]

\[ U_{NO3,t} = \{ U_{wir} [NO_3^-] + 2\pi L_{r,t} D_{NO3} ([NO_3^-] - [NO_3^-]) / \ln(d_{r,t} / r_{r,t,c}) \} \]

\[ = U'_{NO3}(U_{O2r,t} / U'_{O2r,t}) A_{r,t} ([NO_3^-] - [NO_3^-]) / ([NO_3^-] - [NO_3^-]) + K_{NO3} f_{\text{init}} f_{\text{init},r,t} \]

\[ U_{PO4,t} = \{ U_{wir} [H_3PO_4^-] + 2\pi L_{r,t} D_{PO4} ([H_3PO_4^-] - [H_3PO_4^-]) / \ln(d_{r,t} / r_{r,t,c}) \} \]

\[ = U'_{PO4}(U_{O2r,t} / U'_{O2r,t}) A_{r,t} ([H_3PO_4^-] - [H_3PO_4^-]) / ([H_3PO_4^-] - [H_3PO_4^-]) + K_{PO4} f_{\text{init}} f_{\text{init},r,t} \]

\[ f_{\text{init},r,t} = \sigma_{Cl,t} / (\sigma_{Cl,t} + \sigma_{No,t} / KNC) \]

\[ f_{\text{init},r,t} = \sigma_{Cl,t} / (\sigma_{Cl,t} + \sigma_{Pc,t} / KPC) \]

### C4 Gross Primary Productivity

\[ C4PP = \Sigma \{ V_{g(m4)ij,j,k,l,m,n,o} + V_{c(m4)ij,j,k,l,m,n,o} \} \]

\[ V_{g(m4)ij,j,k,l,m,n,o} = (C_o - C_{c(m4)ij,j,k,l,m,n,o}) / r_{r,ijkl,m,n,o} \]

branch growth driven by \( R_g \)  

root growth driven by \( R_g \)  

leaf expansion driven by leaf mass growth  

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

Arrhenius function for \( R_a \)  

temperature function for \( R_m \)  

root N and P uptake from mass flow + diffusion coupled with active uptake of \( NH_4^+ \), \( NO_3^- \) and \( H_3PO_4^- \) constrained by \( O_2 \) uptake, as modelled for microbial N and P uptake in [A26]  

product inhibition of \( U_{NH4}, U_{NO3} \) and \( U_{PO4} \) determined by \( \sigma_N \) and \( \sigma_P \) vs. \( \sigma_C \) in roots  

gaseous diffusion
\[ V_{\text{cm}(m4),i,j,k,l,m,n,o} = \min \{ V_{\text{m}(m4),i,j,k,l,m,n,o}, V_{\text{f}(m4),i,j,k,l,m,n,o} \} \]

\[ r_{\text{f}i,l,j,k,l,m,n,o} = r_{\text{f}i,\text{min},j,k,l,m,n,o} + (r_{\text{f}i,\text{max}} - r_{\text{f}i,\text{min},j,k,l,m,n,o}) e^{(-\beta \varphi_{i,l,j,k,l,m,n,o})} \]

\[ r_{\text{f}i,\text{max},j,k,l,m,n,o} = \left( C_0 - C_{\text{f}(m4)} \right) / V_{\text{f}(m4),i,j,k,l,m,n,o} \]

\[ V_{\text{b}(m4),i,j,k,l,m,n,o} = V_{\text{b}\text{max}(m4),i,j,k,l,m,n,o} \left( C_{\text{cm}(m4),i,j,k,l,m,n,o} - \Gamma_{(m4),i,j,k,l,m,n,o} \right) / \left( C_{\text{cm}(m4),i,j,k,l,m,n,o} + K_{c(m4)} \right) \]

\[ V_{\text{f}(m4),i,j,k,l,m,n,o} = J_{(m4),i,j,k,l,m,n,o} Y_{(m4),i,j,k,l,m,n,o} \]

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

\[ J_{(b4),i,j,k,l,m,n,o} = \left( \varepsilon I_{i,l,m,n,o} + J_{\text{max}(m4),i,j,k} \right) \left( (\varepsilon I_{i,l,m,n,o} + J_{\text{max}(m4),i,j,k})^2 - 4 \alpha \varepsilon I_{i,l,m,n,o} J_{\text{max}(m4),i,j,k} \right)^{0.5} / (2 \alpha) \]

\[ V_{\text{b}\text{max}(m4),i,j,k} = V_{\text{b}\text{max}(m4)} \left[ N_{\text{pept}(m4),i,j,k} \right] N_{\text{i},i,j,k} A_{i,l,m,n,o} f_C(m4),i,j,k f_{\psi}, f_{\beta i} \]

\[ J_{\text{max}(m4),i,j,k} = J_{\text{max}} \left[ N_{\text{chl}(m4),i,j,k} \right] N_{\text{i},i,j,k} A_{i,l,m,n,o} f_C(m4),i,j,k f_{\psi}, f_{\beta i} \]

\[ f_C(m4),i,j,k = 1.0 / (1.0 + (\varepsilon C_{(m4),i,j,k}) / K_{\text{C}(m4)}) \]

\[ f_{\psi}, i,j,k,l,m,n,o = (r_{\text{f}i,\text{min},j,k,l,m,n,o} / r_{\text{f}i,j,k,l,m,n,o})^{0.5} \]

### C₄ Mesophyll-Bundle Sheath Exchange

\[ V_{X_{\text{C}4}(m4),i,j,k,l,m,n,o} = \kappa_X C_{\text{C}4}(m4) \left( \chi C_{\text{C}4}(m4),i,j,k \right) \left( W_{l(i)b4}(i,j,k) - \chi C_{\text{C}4}(b4),i,j,k \right) \left( W_{l(i)b4}(i,j,k) \right) / (W_{l(i)b4}(i,j,k) + W_{l(i)b4}(i,j,k)) \]

\[ V_{X_{\text{C}4}(b4),i,j,k,l,m,n,o} = \kappa_X C_{\text{C}4}(b4) \left( \chi C_{\text{C}4}(b4),i,j,k \right) \left( 1.0 + C_{\text{C}4}(b4),i,j,k / K_{\beta \text{C}4(4)} \right) / (1.0 + C_{\text{C}4}(b4),i,j,k / K_{\beta \text{C}4(4)}) \]

\[ V_{\varphi(b4),i,j,k,l,m,n,o} = \kappa_{\varphi}(b4) \left( C_{\varphi(b4),i,j,k} - C_{\text{C}4(m4),i,j,k} \right) \left( 12 \times 10^{9} \right) W_{l(i)b4}(i,j,k) \]

\[ \delta \chi C_{\text{C}4(m4),i,j,k} / \delta t = \Sigma_{l,m,n,o} C_{\text{C}4(m4),i,j,k,l,m,n,o} \cdot V_{\text{C}4(m4),i,j,k} \]

\[ \delta \chi C_{\text{C}4(b4),i,j,k} / \delta t = \Sigma_{l,m,n,o} C_{\text{C}4(b4),i,j,k,l,m,n,o} \cdot V_{\text{C}4(b4),i,j,k} \]

\[ \delta C_{\text{C}4(b4),i,j,k} / \delta t = V_{\text{C}4(b4),i,j,k} \cdot \Sigma_{l,m,n,o} C_{\text{C}4(b4),i,j,k,l,m,n,o} \]

- mesophyll carboxylation
- CO₂-limited carboxylation
- light-limited carboxylation
- irradiance response function
- PEPc activity
- chlorophyll activity
- C₄ product inhibition
- non-stomatal water limitation
- mesophyll-bundle sheath transfer
- bundle sheath decarboxylation
- bundle sheath-mesophyll leakage
- mesophyll carboxylation products
- bundle sheath carboxylation products
- bundle sheath CO₂ concentration
$C_i$ Bundle Sheath

$V_{(b4)}_{i,j,k,l,m,n,o} = \min \{ V_{(b4)}_{j,k,l,m,n,o}, V_{(j4)}_{j,k,l,m,n,o} \}$  

$V_{(b4)}_{i,j,k} = V_{\text{max}(b4)}_{i,j,k} (C_{C(b4)}_{i,j,k} - \Gamma_{(b4)}_{i,j,k}) / (C_{C(b4)}_{i,j,k} + K_{C(b4)}_{i,j,k})$

$V_{(j4)}_{i,j,k,l,m,n,o} = J_{(b4)}_{i,j,k,l,m,n,o} Y_{(b4)}_{i,j,k}$

$Y_{(b4)}_{i,j,k} = (C_{C(b4)}_{i,j,k} - \Gamma_{(b4)}_{i,j,k}) / (4.5 C_{C(b4)}_{i,j,k} + 10.5 \Gamma_{(b4)}_{i,j,k})$

$J_{(b4)}_{i,j,k,l,m,n,o} = (e I_{l,m,n,o} + J_{\text{max}(b4)}_{i,j,k} - ((e I_{l,m,n,o} + J_{\text{max}(b4)}_{i,j,k})^2 - 4ae I_{l,m,n,o} J_{\text{max}(b4)}_{i,j,k})^{0.5}) / (2a)$

$Y_{(b4)}_{i,j,k} = V_{\text{max}(b4)}_{i,j,k} \left\{ N_{\text{rub}(b4)}_{i,j,k} \right\} N_{l,i,j,k} A_{l,i,j,k} f_{C(l,c)}_{i,j,k} f_{\text{vi}} f_{\text{fi}}$

$J_{\text{max}(b4)}_{i,j,k} = J_{\text{max}} \left\{ N_{\text{ch}(b4)}_{i,j,k} \right\} N_{l,i,j,k} A_{l,i,j,k} f_{C(3,c)}_{i,j,k} f_{\text{vi}} f_{\text{fi}}$

$f_{C(3,c)}_{i,j,k} = \min \{ [v_{l,i,j,k}] / (v_{l,i}) + [\chi_{c3(b4)}_{i,j,k}] / K_{1\text{vi}}, [\pi_{l,i,j,k}] / (\pi_{l,i,j,k}) + [\chi_{c3(b4)}_{i,j,k}] / K_{1\text{fi}} \}$

$Z_{C_{i,j},l,t,c} = g_{c_{i,j},l,t,c} (\sigma_{C_{i,j}} M_{R_{i,l},t,c} - \sigma_{C_{i,j}} M_{B_{i},l,t,c} ) / (M_{R_{i,l},t,c} + M_{B_{i},l,t,c} )$  

$Z_{N_{i,P_{i},j,l,t,c}} = g_{N_{i,P_{i},j,l,t,c}} (\sigma_{N_{i,P_{i}}} \sigma_{C_{i},l,t,c} - \sigma_{N_{i,P_{i}}} \sigma_{C_{i},l,t,c} ) / (\sigma_{C_{i},l,t,c} + \sigma_{C_{i},l,t,c} )$

$Z_{C_{i,j},l,t,c} = g_{C_{i,j},l,t,c} (\sigma_{C_{i},l,t,c} M_{M_{R_{i},l},t,c} - \sigma_{C_{i},l,t,c} M_{R_{i},l,t,c} ) / (M_{M_{R_{i},l},t,c} + M_{R_{i},l,t,c})$

$Z_{N_{i,P_{i},j,l,t,c}} = g_{N_{i,P_{i},j,l,t,c}} (\sigma_{N_{i,P_{i},j,l,t,c}} \sigma_{C_{i},l,t,c} - \sigma_{N_{i,P_{i},j,l,t,c}} \sigma_{C_{i},l,t,c} ) / (\sigma_{C_{i},l,t,c} + \sigma_{C_{i},l,t,c} )$

**Definition of Variables in Section C**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Unit</th>
<th>Equation</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>species or functional type: evergreen, coniferous, deciduous, annual, perennial, C3, C4, monocot, dicot, legume etc.</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$j$</td>
<td>branch or tiller</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$k$</td>
<td>node</td>
<td></td>
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</tbody>
</table>

**unit**

**subscripts**

bundle sheath carboxylation  
CO$_2$-limited carboxylation  
light- limited carboxylation  
carboxylation efficiency of $V_{(b4)}$  
irradiance response function  
RuBPC activity  
chlorophyll activity  
C$_3$ product inhibition  
shoot – root C transfer driven by $\sigma_C$ concentration gradients  
shoot – root N,P transfer driven by $\sigma_{N,P}$ concentration gradients  
root – mycorrhizal C transfer driven by $\sigma_C$ conc’n gradients  
root – mycorrhizal N,P transfer driven by $\sigma_{N,P}$ conc’n gradients
### Variables

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>$l$</td>
<td>soil or canopy layer</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m$</td>
<td>leaf azimuth</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>leaf inclination</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$o$</td>
<td>leaf exposure (sunlit vs. shaded)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$z$</td>
<td>organ including leaf, stem, root $r$, mycorrhizae $m$</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>leaf, root or mycorrhizal surface area</td>
<td>$m^2$</td>
<td>[C1, C6b, C6d, C8b, C21, C23, C32, C33, C47]</td>
</tr>
<tr>
<td>$\beta$</td>
<td>shape parameter for stomatal effects on CO$_2$ diffusion and non-stomatal effects on carboxylation</td>
<td>MPa$^{-1}$</td>
<td>[C4, C27, C35, -5.0]</td>
</tr>
<tr>
<td>$B_j$</td>
<td>parameter such that $f_{j_0} = 1.0$ at $T_c = 298.15$ K</td>
<td></td>
<td>[C10c] 17.354</td>
</tr>
<tr>
<td>$B_{ke}$</td>
<td>parameter such that $f_{ke_3} = 1.0$ at $T_c = 298.15$ K</td>
<td></td>
<td>[C10d] 22.187</td>
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<tr>
<td>$B_{ko}$</td>
<td>parameter such that $f_{ko_3} = 1.0$ at $T_c = 298.15$ K</td>
<td></td>
<td>[C10e] 8.067</td>
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<tr>
<td>$B_o$</td>
<td>parameter such that $f_{o_3} = 1.0$ at $T_c = 298.15$ K</td>
<td></td>
<td>[C10b] 24.212</td>
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<tr>
<td>$B_v$</td>
<td>parameter such that $f_{v_3} = 1.0$ at $T_c = 298.15$ K</td>
<td></td>
<td>[C10a, C22] 26.229</td>
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<tr>
<td>$C_b$</td>
<td>[CO$_2$] in canopy air</td>
<td>$\mu$mol mol$^{-1}$</td>
<td>[C2, C5, C25, C28]</td>
</tr>
<tr>
<td>$C_c$</td>
<td>[CO$<em>2$] in canopy chloroplasts in equilibrium with $C</em>{i,j,k,l,m,n,o}$</td>
<td>$\mu$M</td>
<td>[C6a, C7b]</td>
</tr>
<tr>
<td>$C_{(b4)}$</td>
<td>[CO$_2$] in C$_4$ bundle sheath</td>
<td>$\mu$M</td>
<td>[C38, C39, C42, C44, C45b]</td>
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<tr>
<td>$C_{(m4)}$</td>
<td>[CO$_2$] in C$<em>4$ mesophyll in equilibrium with $C</em>{i,j,k,l,m,n,o}$</td>
<td>$\mu$M</td>
<td>[C29, C30b, C39]</td>
</tr>
<tr>
<td>$C'_i$</td>
<td>[CO$<em>2$] in canopy leaves when $\psi</em>{ij} = 0$</td>
<td>$\mu$mol mol$^{-1}$</td>
<td>[C5] 0.70 x $C_b$</td>
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<tr>
<td>$C_i$</td>
<td>[CO$_2$] in canopy leaves</td>
<td>$\mu$mol mol$^{-1}$</td>
<td>[C2]</td>
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<tr>
<td>$C_{(m4)}'$</td>
<td>[CO$_2$] in C$<em>4$ mesophyll air when $\psi</em>{ij} = 0$</td>
<td>$\mu$mol mol$^{-1}$</td>
<td>[C28] 0.45 x $C_b$</td>
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</tbody>
</table>
### Table of Symbols and Units

<table>
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<th>Symbol</th>
<th>Description</th>
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<th>Reference</th>
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<tbody>
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<td>$C_{i(m4)}$</td>
<td>[CO$_2$] in C$_4$ mesophyll air</td>
<td>µmol mol$^{-1}$</td>
<td>C25</td>
</tr>
<tr>
<td>$C_{i,z=l}$</td>
<td>C content of leaf ($z = l$)</td>
<td>g C m$^{-2}$</td>
<td>C18</td>
</tr>
<tr>
<td>$D_{e \text{NH}_{4l}}$</td>
<td>effective dispersivity-diffusivity of NH$_4^+$ during root uptake</td>
<td>m$^2$ h$^{-1}$</td>
<td>C23</td>
</tr>
<tr>
<td>$D_{e \text{NO}_{3l}}$</td>
<td>effective dispersivity-diffusivity of NO$_3^-$ during root uptake</td>
<td>m$^2$ h$^{-1}$</td>
<td>C23</td>
</tr>
<tr>
<td>$D_{e \text{H}_2\text{PO}_4l}$</td>
<td>effective dispersivity-diffusivity of H$_2$PO$_4^-$ during root uptake</td>
<td>m$^2$ h$^{-1}$</td>
<td>C23</td>
</tr>
<tr>
<td>$D_{\text{O}_2}$</td>
<td>aqueous diffusivity of O$_2$ from root aerenchyma to root or mycorrhizal surfaces</td>
<td>m$^2$ h$^{-1}$</td>
<td>C14d</td>
</tr>
<tr>
<td>$D_{\text{O}_2}$</td>
<td>aqueous diffusivity of O$_2$ from soil to root or mycorrhizal surfaces</td>
<td>m$^2$ h$^{-1}$</td>
<td>C14d</td>
</tr>
<tr>
<td>$d_{i,r,l}$</td>
<td>half distance between adjacent roots assumed equal to uptake path length</td>
<td>m</td>
<td>C23</td>
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<tr>
<td>$E_{N,P}$</td>
<td>energy cost of nutrient uptake</td>
<td>g C g N$^{-1}$ or P$^{-1}$</td>
<td>C13, 2.15 Veen (1981)</td>
</tr>
<tr>
<td>$f_{C_{(c3)}}$</td>
<td>C$_3$ product inhibition of RuBP carboxylation activity in C$_4$ bundle sheath or C$_3$ mesophyll</td>
<td>–</td>
<td>C47,C48,C49</td>
</tr>
<tr>
<td>$f_{C_{(m4)}}$</td>
<td>C$_4$ product inhibition of PEP carboxylation activity in C$_4$ mesophyll</td>
<td>–</td>
<td>C32,C33,C34</td>
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<tr>
<td>$F_{\text{chl}}$</td>
<td>fraction of leaf protein in chlorophyll</td>
<td>-</td>
<td>C8b 0.025</td>
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<tr>
<td>$f_{IC}$</td>
<td>N,P inhibition on carboxylation, leaf structural N,P growth</td>
<td>–</td>
<td>C6a,C7,C11,C12</td>
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<tr>
<td>$f_{IN}$</td>
<td>N inhibition on root N uptake</td>
<td>–</td>
<td>C23g</td>
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<tr>
<td>$f_{IP}$</td>
<td>P inhibition on root P uptake</td>
<td>–</td>
<td>C23h</td>
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<tr>
<td>$f_{\phi_N}$</td>
<td>fraction of $X_{\text{mx}}$ N translocated out of leaf or root before litterfall</td>
<td>–</td>
<td>C19a,c</td>
</tr>
<tr>
<td>$f_{\phi_P}$</td>
<td>fraction of $X_{\text{mx}}$ P translocated out of leaf or root before litterfall</td>
<td>–</td>
<td>C19b,d</td>
</tr>
</tbody>
</table>
$F_{rubisco}$ fraction of leaf protein in rubisco $-$ [C6b,d] 0.125

$f_{ta}$ temperature effect on $R_{m,i,j}$ and $U$ $-$ [C14,C22,C23] Bernacchi et al. (2001,2003)

$f_{tb}$ temperature effect on carboxylation $-$ [C6b,C10a] Bernacchi et al. (2001,2003)

$f_{tj}$ temperature effect on electron transport $-$ [C8b,C10c] Bernacchi et al. (2001,2003)

$f_{tkc}$ temperature effect on $K_{ci}$ $-$ [C6e,C10d] Bernacchi et al. (2001,2003)

$f_{tko}$ temperature effect on $K_{oi}$ $-$ [C6e,C10c] Bernacchi et al. (2001,2003)

$f_{tm}$ temperature effect on $R_{mi,j}$ $-$ [C16, C22b] $Q_{10} = 2.25$

$f_{to}$ temperature effect on oxygenation $-$ [C6d,C22b] Bernacchi et al. (2001,2003)


$f_{xN}$ inhibition of root or mycorrhizal N exudation $-$ [C19f,h] Medrano et al. (2002)

$f_{xP}$ inhibition of root or mycorrhizal P exudation $-$ [C19g,i] Medrano et al. (2002)

$f_{xj}$ non-stomatal water effect on carboxylation $-$ [C6a,C7a,C9] Bernacchi et al. (2001,2003)


$g_{sC}$ conductance for shoot-root C transfer $h^{-1}$ [C50] calculated from root depth, axis number

$g_{sNP}$ rate constant for shoot-root N,P transfer $h^{-1}$ [C51] 0.1 Grant (1998)

$g_{rC}$ rate constant for root-mycorrhizal C transfer $h^{-1}$ [C52] 0.1 Grant (1998)

$g_{rNP}$ rate constant for root-mycorrhizal N,P transfer $h^{-1}$ [C53] 0.1 Grant (1998)

$H_{aj}$ energy of activation for electron transport $J \text{ mol}^{-1}$ [C10c] $43 \times 10^3$ Bernacchi et al. (2001,2003)
$H_{hko}$ parameter for temperature sensitivity of $K_{ci}$ $J \text{ mol}^{-1}$ [C10d] 55 x 10$^3$ Bernacchi et al. (2001, 2003)

$H_{hko}$ parameter for temperature sensitivity of $K_{oi}$ $J \text{ mol}^{-1}$ [C10e] 20 x 10$^3$ Bernacchi et al. (2001, 2003)

$H_{ao}$ energy of activation for oxygenation $J \text{ mol}^{-1}$ [C10b, C22] 60 x 10$^3$ Bernacchi et al. (2001, 2003)

$H_{av}$ energy of activation for carboxylation $J \text{ mol}^{-1}$ [C10a, C22] 65 x 10$^3$ Bernacchi et al. (2001, 2003)

$H_{dh}$ energy of high temperature deactivation $J \text{ mol}^{-1}$ [C10, C22] 222.5 x 10$^3$ Bernacchi et al. (2001, 2003)

$H_{dl}$ energy of low temperature deactivation $J \text{ mol}^{-1}$ [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]

$[H_2PO_4]_{i,m}$ 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 $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C8a, C8b]

$J$ electron transport rate in $C_3$ mesophyll $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C7a, C8a]

$J_{(b4)}$ electron transport rate in $C_4$ bundle sheath $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C45a, C46]

$J_{(m4)}$ electron transport rate in $C_4$ mesophyll $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C30a, C31]

$J_{max'}$ specific electron transport rate at non-limiting $I$ and 25$^\circ$C when $\psi_{ci} = 0$ and nutrients are nonlimiting $\mu\text{mol g}^{-1} \text{s}^{-1}$ [C33, C48] 400

$J_{max(b4)}$ electron transport rate in $C_4$ bundle sheath at non-limiting $I$ $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C46, C48]

$J_{max(m4)}$ electron transport rate in $C_4$ mesophyll at non-limiting $I$ $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C31, C33]

$J_{max}$ electron transport rate at non-limiting $I$, $\psi_{ci}$, temperature and N, P $\mu\text{mol m}^{-2} \text{s}^{-1}$ [C8a, C8b]

$K_{c(b4)}$ Michaelis-Menten constant for carboxylation in $C_4$ bundle sheath $\mu\text{M}$ [C44] 30.0 at 25$^\circ$C and zero $O_2$ Lawlor (1993)

$K_{c(m4)}$ Michaelis-Menten constant for carboxylation in $C_4$ mesophyll $\mu\text{M}$ [C29] 3.0 at 25$^\circ$C Lawlor (1993)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
<th>Source</th>
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<tbody>
<tr>
<td>$K_c$</td>
<td>Michaelis-Menten constant for carboxylation at zero $O_2$</td>
<td>$\mu M$</td>
<td>$[C6c,C6e]$</td>
<td>12.5 at 25 °C</td>
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<tr>
<td>$K_c$</td>
<td>Michaelis-Menten constant for carboxylation at ambient $O_2$</td>
<td>$\mu M$</td>
<td>$[C6e]$</td>
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<tr>
<td>$K_{ICN}$</td>
<td>inhibition constant for growth in shoots from $\sigma_C$ vs. $\sigma_N$</td>
<td>$g C g N^{-1}$</td>
<td>$[C11]$</td>
<td>100</td>
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<tr>
<td>$K_{ICP}$</td>
<td>inhibition constant for growth in shoots from $\sigma_C$ vs. $\sigma_P$</td>
<td>$g C g P^{-1}$</td>
<td>$[C11]$</td>
<td>1000</td>
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<tr>
<td>$K_{IC(C4b4)}$</td>
<td>constant for CO$_2$ product inhibition of C$_4$ decarboxylation in C$_4$ bundle sheath</td>
<td>$\mu M$</td>
<td>$[C38]$</td>
<td>1000.0</td>
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<tr>
<td>$K_{IC(C4mes)}$</td>
<td>constant for C$_4$ product inhibition of PEP carboxylation activity in C$_4$ mesophyll</td>
<td>$\mu M$</td>
<td>$[C34]$</td>
<td>$5 \times 10^6$</td>
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<tr>
<td>$K_{IC(C3)}$</td>
<td>constant for C$_3$ product inhibition of RuBP carboxylation activity in C$_4$ bundle sheath or C$<em>3$ mesophyll caused by $[\pi</em>{i,j}]$</td>
<td>$g C g N^{-1}$</td>
<td>$[C49]$</td>
<td>100</td>
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<tr>
<td>$K_{IC(C3)}$</td>
<td>constant for C$_3$ product inhibition of RuBP carboxylation activity in C$_4$ bundle sheath or C$<em>3$ mesophyll caused by $[\alpha</em>{i,j}]$</td>
<td>$g C g P^{-1}$</td>
<td>$[C49]$</td>
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<tr>
<td>$K_{ICN}$</td>
<td>inhibition constant for N uptake in roots from $\sigma_{C,i,j}$ vs. $\sigma_{N,j}$</td>
<td>$g N g C^{-1}$</td>
<td>$[C23]$</td>
<td>0.1</td>
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<tr>
<td>$K_{ICP}$</td>
<td>inhibition constant for P uptake in roots from $\sigma_{C,i,j}$ vs. $\sigma_{P,j}$</td>
<td>$g P g C^{-1}$</td>
<td>$[C23]$</td>
<td>0.01</td>
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<tr>
<td>$K_{IN}$</td>
<td>inhibition constant for remobilization of leaf or root N during senescence</td>
<td>$g N g C^{-1}$</td>
<td>$[C19c]$</td>
<td>0.1</td>
</tr>
<tr>
<td>$K_{IP}$</td>
<td>inhibition constant for remobilization of leaf or root P during senescence</td>
<td>$g P g C^{-1}$</td>
<td>$[C19d]$</td>
<td>0.01</td>
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<tr>
<td>$K_{NH4}$</td>
<td>M-M constant for NH$_4^+$ uptake at root or mycorrhizal surfaces</td>
<td>$g N m^{-3}$</td>
<td>$[C23]$</td>
<td>0.40</td>
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<tr>
<td>$K_{NO3}$</td>
<td>M-M constant for NO$_3^-$ uptake at root or mycorrhizal surfaces</td>
<td>$g N m^{-3}$</td>
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<tr>
<td>$K_{PO4}$</td>
<td>M-M constant for H$_2$PO$_4^-$ uptake at root or mycorrhizal surfaces</td>
<td>$g P m^{-3}$</td>
<td>$[C23]$</td>
<td>0.125</td>
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<tr>
<td>$K_{O2}$</td>
<td>Michaelis-Menten constant for root or mycorrhizal $O_2$ uptake</td>
<td>$g m^{-3}$</td>
<td>$[C14c]$</td>
<td>0.32</td>
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<td>Reference</td>
<td>Additional Information</td>
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<td>$K_o$</td>
<td>inhibition constant for $O_2$ in carboxylation</td>
<td>$\mu$M</td>
<td>[C6c,C6e] 500 at 25 °C</td>
<td>Farquhar et al. (1980)</td>
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<tr>
<td>$K_{xN}$</td>
<td>inhibition constant for exudation of root or mycorrhizal N</td>
<td>g C g N$^{-1}$</td>
<td>[C19h] 1.0</td>
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<tr>
<td>$K_{xP}$</td>
<td>inhibition constant for exudation of root or mycorrhizal P</td>
<td>g C g N$^{-1}$</td>
<td>[C19i] 10.0</td>
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<tr>
<td>$L$</td>
<td>root length</td>
<td>m m$^{-2}$</td>
<td>[C14d,C21b,C23]</td>
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<tr>
<td>$l_C$</td>
<td>C litterfall from leaf or root</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C18,C19a,b,C20]</td>
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<tr>
<td>$l_{N,P}$</td>
<td>N or P litterfall from leaf or root</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C19a,b]</td>
<td></td>
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<tr>
<td>$M_B$</td>
<td>branch C phytomass</td>
<td>g C m$^{-2}$</td>
<td>[C20,C50]</td>
<td></td>
</tr>
<tr>
<td>$M_L$</td>
<td>leaf C phytomass</td>
<td>g C m$^{-2}$</td>
<td>[C12,C21]</td>
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<tr>
<td>$M_{N^*,R}$</td>
<td>non-remobilizable, remobilizable (protein) leaf C phytomass</td>
<td>g C m$^{-2}$</td>
<td>[C12,C18]</td>
<td></td>
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<tr>
<td>$M_M$</td>
<td>mycorrhizal C phytomass</td>
<td>g C m$^{-2}$</td>
<td>[C52]</td>
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<tr>
<td>$M_R$</td>
<td>root C phytomass</td>
<td>g C m$^{-2}$</td>
<td>[C20,C21,C50,C52]</td>
<td></td>
</tr>
<tr>
<td>$M_{prot}$</td>
<td>leaf protein phytomass calculated from leaf N, P contents</td>
<td>g N m$^{-2}$</td>
<td>[C6b,C6d,C8b]</td>
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<tr>
<td>N,P</td>
<td>N or P content of organ $z$</td>
<td>g N m$^{-2}$</td>
<td>[C16, C19]</td>
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</tr>
<tr>
<td>$N_{leaf}$</td>
<td>maximum leaf structural N content</td>
<td>g N g C$^{-1}$</td>
<td>[C12] 0.10</td>
<td></td>
</tr>
<tr>
<td>$N'_{leaf}$</td>
<td>minimum leaf structural N content</td>
<td>g N g C$^{-1}$</td>
<td>[C12] 0.33 x $N_{leaf}$</td>
<td></td>
</tr>
<tr>
<td>$N_{lf}$</td>
<td>total leaf N</td>
<td>g N m$^{-2}$ leaf</td>
<td>[C32,C33,C47,C48]</td>
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</tr>
<tr>
<td>$N_{prot}$</td>
<td>N content of protein remobilized from leaf or root</td>
<td>g N C$^{-1}$</td>
<td>[C12,C19a] 0.4</td>
<td></td>
</tr>
<tr>
<td>$[N_{chlo(b)}]'$</td>
<td>ratio of chlorophyll N in C$_4$ bundle sheath to total leaf N</td>
<td>g N g N$^{-1}$</td>
<td>[C48] 0.05</td>
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</tr>
<tr>
<td>$[N_{chlo(m)}]'$</td>
<td>ratio of chlorophyll N in C$_4$ mesophyll to total leaf N</td>
<td>g N g N$^{-1}$</td>
<td>[C33] 0.05</td>
<td></td>
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</tbody>
</table>
[\text{NH}_4^{+}]_{\text{rr,tl}} \quad \text{concentration of NH}_4^+ \text{ at root or mycorrizal surfaces} \quad \text{g N m}^{-3} \quad \text{[C23]}

[\text{NH}_4^{+}]_{\text{mn}} \quad \text{concentration of NH}_4^+ \text{ at root or mycorrizal surfaces below which } U_{\text{NH}_4} = 0 \quad \text{g N m}^{-3} \quad \text{[C23]}

[\text{NO}_3^-]_{\text{rr,tl}} \quad \text{concentration of NH}_4^+ \text{ at root or mycorrizal surfaces} \quad \text{g N m}^{-3} \quad \text{[C23]}

[\text{NO}_3^-]_{\text{mn}} \quad \text{concentration of NO}_3^- \text{ at root or mycorrizal surfaces below which } U_{\text{NO}_3} = 0 \quad \text{g N m}^{-3} \quad \text{[C23]}

\text{Barber and Silberbush, 1984}

[\text{NO}_3^-]_{\text{mr,tl}} \quad \text{concentration of NO}_3^- \text{ at root or mycorrizal surfaces} \quad \text{g N m}^{-3} \quad \text{[C23]}

\text{Barber and Silberbush, 1984}

\text{[N}_{\text{pep(})_{\text{mr,tl}} \quad \text{ratio of PEP carboxylase N in C}_4 \text{ mesophyll to total leaf N} \quad \text{g N g N}^{-1} \quad \text{[C32]}

\text{[N}_{\text{rub(b)}}_{\text{mr,tl}} \quad \text{ratio of RuBP carboxylase N in C}_4 \text{ bundle sheath to total leaf N} \quad \text{g N g N}^{-1} \quad \text{[C47]}

\text{O}_{2q} \quad \text{aqueous O}_2 \text{ concentration in root or mycorrhizal aerenchyma} \quad \text{g m}^{-3} \quad \text{[C14c,d]}

\text{O}_{2r} \quad \text{aqueous O}_2 \text{ concentration at root or mycorrhizal surfaces} \quad \text{g m}^{-3} \quad \text{[C14c,d]}

\text{O}_{2s} \quad \text{aqueous O}_2 \text{ concentration in soil solution} \quad \text{g m}^{-3} \quad \text{[C14c,d]}

\text{O}_c \quad [\text{O}_2] \text{ in canopy chloroplasts in equilibrium with O}_2 \text{ in atm.} \quad \text{µM} \quad \text{[C6c,C6e]}

\text{P}_{\text{leaf}} \quad \text{maximum leaf structural P content} \quad \text{g P g C}^{-1} \quad \text{[C12]}

\text{P'}_{\text{leaf}} \quad \text{minimum leaf structural P content} \quad \text{g P g C}^{-1} \quad \text{[C12]}

\text{0.33 x P}_{\text{leaf}}

\text{P}_{\text{prot}} \quad \text{P content of protein remobilized from leaf or root} \quad \text{g P C}^{-1} \quad \text{[C12,C19b]}

\text{0.04}

[\sigma_{\text{ml}}] \quad \text{concentration of nonstructural root P uptake product in leaf} \quad \text{g P g C}^{-1} \quad \text{[C49]}

\text{0.1 – 0.5}

\text{0.015}

\text{0.025}

\text{0.025}

\text{[C10, C22]}

8.3143

\text{J mol}^{-1} \text{K}^{-1}
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Reference</th>
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</thead>
<tbody>
<tr>
<td>$R_c$</td>
<td>autotrophic respiration of $\sigma_{C_{ij}}$ or $\sigma_{C_{ir,l}}$</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C13,C14,C17,C15]</td>
</tr>
<tr>
<td>$R_g$</td>
<td>growth respiration</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C17,C20]</td>
</tr>
<tr>
<td>$r_{lf}$</td>
<td>leaf stomatal resistance</td>
<td>s m$^{-1}$</td>
<td>[C25,C27,C39]</td>
</tr>
<tr>
<td>$r_{lf\text{maxi}}$</td>
<td>leaf cuticular resistance</td>
<td>s m$^{-1}$</td>
<td>[C27]</td>
</tr>
<tr>
<td>$r_{lf\text{mini,j,k,l,m,n,o}}$</td>
<td>leaf stomatal resistance when $\psi_{ci} = 0$</td>
<td>s m$^{-1}$</td>
<td>[C27,C28,C35]</td>
</tr>
<tr>
<td>$r_{li,j,k,l,m,n,o}$</td>
<td>leaf stomatal resistance</td>
<td>s m$^{-1}$</td>
<td>[C2,C4,C9]</td>
</tr>
<tr>
<td>$r_{li\text{maxi}}$</td>
<td>leaf cuticular resistance</td>
<td>s m$^{-1}$</td>
<td>[C4]</td>
</tr>
<tr>
<td>$r_{li\text{mini,j,k,l,m,n,o}}$</td>
<td>leaf stomatal resistance when $\psi_{ci} = 0$</td>
<td>s m$^{-1}$</td>
<td>[C4,C5,C9]</td>
</tr>
<tr>
<td>$R_{m'}$</td>
<td>specific maintenance respiration of $\sigma_{C_{ij}}$ at $T_{ci} = 25$°C</td>
<td>g C g N$^{-1}$ h$^{-1}$</td>
<td>[C16]</td>
</tr>
<tr>
<td>$R_{m_{ij}}$</td>
<td>above-ground maintenance respiration</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C16,C17,C15]</td>
</tr>
<tr>
<td>$r_{q,r,l}$</td>
<td>radius of root aerenchyma</td>
<td>m</td>
<td>[C14d]</td>
</tr>
<tr>
<td>$r_{r,l}$</td>
<td>root or mycorrhizal radius</td>
<td>m</td>
<td>[C14d,C21b,c,C23a,c,e]</td>
</tr>
<tr>
<td>$R_{s_{ij}}$</td>
<td>respiration from remobilization of leaf C</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C13,C15,C18,C20]</td>
</tr>
<tr>
<td>$r_{sl}$</td>
<td>thickness of soil water films</td>
<td>m</td>
<td>[C14d]</td>
</tr>
<tr>
<td>$r_x$</td>
<td>rate constant for root or mycorrhizal exudation</td>
<td>h$^{-1}$</td>
<td>[C19f,g,h]</td>
</tr>
<tr>
<td>$\rho_r$</td>
<td>dry matter content of root biomass</td>
<td>g g$^{-1}$</td>
<td>[C21b]</td>
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<tr>
<td>$S$</td>
<td>change in entropy</td>
<td>J mol$^{-1}$ K$^{-1}$</td>
<td>[C10,C22]</td>
</tr>
<tr>
<td>$\sigma_C$</td>
<td>nonstructural C product of CO$_2$ fixation</td>
<td>g C g$^{-1}$</td>
<td>[C11,C19c,d,e,h,i,C23g,h,C50-53]</td>
</tr>
</tbody>
</table>
\( \sigma_N \) nonstructural N product of root uptake \( g \, N \, g^{-1} \, C \) [C11, C19c,f,h,i C23g,h,C51,C53]

\( \sigma_P \) nonstructural P product of root uptake \( g \, P \, g^{-1} \, C \) [C11, C19d,g,h,i C23g,h,C51,C53]

\( T_c \) canopy temperature \( K \) [C10, C22]

\( U'_{NH4,c,r,l} \) \( NH_4^+ \) uptake by roots or mycorrhizae \( g \, N \, m^{-2} \, h^{-1} \) [C23]

\( U'_{NO3,c,r,l} \) maximum \( U_{NO3} \) at 25 °C and non-limiting \( NO_3^- \) \( g \, N \, m^{-2} \, h^{-1} \) [C23] 5.0 x 10^{-3} Barber and Silberbush, 1984

\( U'_{PO4,c,r,l} \) \( H_2PO_4^- \) uptake by roots or mycorrhizae \( g \, N \, m^{-2} \, h^{-1} \) [C23]

\( U'_{O2,c,r,l} \) \( O_2 \) uptake by roots and mycorrhizae under ambient \( O_2 \) \( g \, O \, m^{-2} \, h^{-1} \) [C14b,c,C23b,d,f]

\( U'_{CO2,c,r,l} \) \( O_2 \) uptake by roots and mycorrhizae under nonlimiting \( O_2 \) \( g \, O \, m^{-2} \, h^{-1} \) [C14b,c,C23b,d,f]

\( U_{w,c,r,l} \) root water uptake \( m^3 \, m^{-2} \, h^{-1} \) [C14d,C23]

\( V_{gb4v,j,k} \) \( CO_2 \) leakage from \( C_4 \) bundle sheath to \( C_4 \) mesophyll \( g \, C \, m^2 \, h^{-1} \) [C39,C42]

\( V'_b \) specific rubisco carboxylation at 25 °C \( \mu mol \, g^{-1} \, rubisco \, s^{-1} \) [C6b] 45 Farquhar et al. (1980)

\( V_{b4v4v,j,k} \) \( CO_2 \)-limited carboxylation rate in \( C_4 \) bundle sheath \( \mu mol \, m^2 \, s^{-1} \) [C43,C44]

\( V_{b4v4v,j,k,m,n,o} \) \( CO_2 \)-limited carboxylation rate in \( C_4 \) mesophyll \( \mu mol \, m^2 \, s^{-1} \) [C26]

\( V_{b4v4v,j,k,m,n,o} \) \( CO_2 \)-limited leaf carboxylation rate \( \mu mol \, m^2 \, s^{-1} \) [C3,C6]

\( V_{bmax(b4)}' \) RuBP carboxylase specific activity in \( C_4 \) bundle sheath at 25°C when \( \varphi_c = 0 \) and nutrients are nonlimiting \( \mu mol \, g^{-1} \, s^{-1} \) [C47] 75
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<td>( V_{\text{bmax}(b4)i,j,k} )</td>
<td>CO(_2)-nonlimited carboxylation rate in C(_4) bundle sheath</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C44,C47]</td>
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<td>( V_{\text{bmax}(m4)}' )</td>
<td>PEP carboxylase specific activity in C(<em>4) mesophyll at 25(^\circ)C when ( \psi</em>{ci} = 0 ) and nutrients are nonlimiting</td>
<td>( \mu \text{mol g}^{-1} \text{s}^{-1} )</td>
<td>[C32]</td>
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<tr>
<td>( V_{\text{bmax}(m4)i,j,k} )</td>
<td>CO(_2)-nonlimited carboxylation rate in C(_4) mesophyll</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C29,C32]</td>
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<tr>
<td>( V_{\text{bmax}(i,j,k)} )</td>
<td>leaf carboxylation rate at non-limiting ( \text{CO}<em>2 ), ( \psi</em>{ci} ), ( T_c ) and N,P</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C6a,C6b,C6c]</td>
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<td>( V_{(b4)i,j,k,l,m,n,o} )</td>
<td>( \text{CO}_2 ) fixation rate in C(_4) bundle sheath</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C43]</td>
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<tr>
<td>( V_{(m4)i,j,k,l,m,n,o} )</td>
<td>( \text{CO}_2 ) fixation rate in C(_4) mesophyll</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C24,C26,C40,C41]</td>
</tr>
<tr>
<td>( V_{(m4)i,j,k,l,m,n,o} )</td>
<td>( \text{CO}_2 ) fixation rate in C(<em>4) mesophyll when ( \psi</em>{ci} = 0 ) MPa</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C28]</td>
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<tr>
<td>( V_{i,j,k,l,m,n,o} )</td>
<td>leaf ( \text{CO}_2 ) fixation rate</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C1,C3]</td>
</tr>
<tr>
<td>( V_{c(i,j,k,l,m,n,o)} )</td>
<td>leaf ( \text{CO}<em>2 ) fixation rate when ( \psi</em>{ci} = 0 )</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C5]</td>
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<tr>
<td>( V_{g(m4)i,j,k,l,m,n,o} )</td>
<td>( \text{CO}_2 ) diffusion rate into C(_4) mesophyll</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C24,C25]</td>
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<tr>
<td>( V_{g(i,j,k,l,m,n,o)} )</td>
<td>leaf ( \text{CO}_2 ) diffusion rate</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C1,C2]</td>
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<td>( V_{j}' )</td>
<td>specific chlorophyll e` transfer at 25 (^\circ)C</td>
<td>( \mu \text{mol g}^{-1} \text{chlorophyll s}^{-1} )</td>
<td>[C8b]</td>
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<td>( V_{j(b4)i,j,k,l,m,n,o} )</td>
<td>irradiance-limited carboxylation rate in C(_4) bundle sheath</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C43,C45a]</td>
</tr>
<tr>
<td>( V_{j(m4)i,j,k,l,m,n,o} )</td>
<td>irradiance-limited carboxylation rate in C(_4) mesophyll</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C26,C30a]</td>
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<tr>
<td>( V_{j(i,j,k,l,m,n,o)} )</td>
<td>irradiance-limited leaf carboxylation rate</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C3,C7a]</td>
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<tr>
<td>( V_{o}' )</td>
<td>specific rubisco oxygenation at 25 (^\circ)C</td>
<td>( \mu \text{mol g}^{-1} \text{rubisco s}^{-1} )</td>
<td>[C6d]</td>
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<tr>
<td>( V_{o_{\text{max},i,j,k}} )</td>
<td>leaf oxygenation rate at non-limiting ( \text{O}<em>2 ), ( \psi</em>{ci} ), ( T_c ) and N,P</td>
<td>( \mu \text{mol m}^{-2} \text{s}^{-1} )</td>
<td>[C6c,d]</td>
</tr>
<tr>
<td>( V_{j(\text{C4})b4(i,j,k)} )</td>
<td>decarboxylation of C(_4) fixation product in C(_4) bundle sheath</td>
<td>g C m(^{-2}) h(^{-1})</td>
<td>[C38,C41,C42]</td>
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</tbody>
</table>

*Farquhar et al. (1980)*
<table>
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<th>Symbol</th>
<th>Definition</th>
<th>Units</th>
<th>Reference</th>
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<tr>
<td>$V_{C4(m4)}$</td>
<td>transfer of C\textsubscript{4} fixation product between C\textsubscript{4} mesophyll and</td>
<td>g m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C37]</td>
</tr>
<tr>
<td>$[\nu_l]$</td>
<td>concentration of nonstructural root N uptake product in leaf</td>
<td>g N g C\textsuperscript{-1}</td>
<td>[C49]</td>
</tr>
<tr>
<td>$v_r$</td>
<td>specific volume of root biomass</td>
<td>m\textsuperscript{3} g\textsuperscript{-1}</td>
<td>[C21b]</td>
</tr>
<tr>
<td>$W_{f(b4)}$</td>
<td>C\textsubscript{4} bundle sheath water content</td>
<td>g m\textsuperscript{2}</td>
<td>[C37,C39]</td>
</tr>
<tr>
<td>$W_{f(m4)}$</td>
<td>C\textsubscript{4} mesophyll water content</td>
<td>g m\textsuperscript{2}</td>
<td>[C37]</td>
</tr>
<tr>
<td>$X_{mx}$</td>
<td>maximum fraction of remobilizable N or P translocated out of leaf or root during senescence</td>
<td>-</td>
<td>[C19a,b]</td>
</tr>
<tr>
<td>$x_{i,r,l,C}$</td>
<td>root and mycorrhizal C exudation</td>
<td>g C m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C19e]</td>
</tr>
<tr>
<td>$x_{i,r,l,N}$</td>
<td>root and mycorrhizal C exudation</td>
<td>g N m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C19f]</td>
</tr>
<tr>
<td>$x_{i,r,l,P}$</td>
<td>root and mycorrhizal C exudation</td>
<td>g P m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C19g]</td>
</tr>
<tr>
<td>$Y$</td>
<td>carboxylation yield from electron transport in C\textsubscript{3} mesophyll</td>
<td>\mu mol CO\textsubscript{2} \mu mol e\textsuperscript{-1}</td>
<td>[C7a,b]</td>
</tr>
<tr>
<td>$Y_{(b4)}$</td>
<td>carboxylation yield from electron transport in C\textsubscript{4} bundle sheath</td>
<td>\mu mol CO\textsubscript{2} \mu mol e\textsuperscript{-1}</td>
<td>[C45a,b]</td>
</tr>
<tr>
<td>$Y_{(m4)}$</td>
<td>carboxylation yield from electron transport in C\textsubscript{4} mesophyll</td>
<td>\mu mol CO\textsubscript{2} \mu mol e\textsuperscript{-1}</td>
<td>[C30a,b]</td>
</tr>
<tr>
<td>$Y_g$</td>
<td>fraction of $\sigma_{Ci,j}$ used for growth expended as $R_{g(i,z)}$ by organ (z)</td>
<td>g C g C\textsuperscript{-1}</td>
<td>[C20]</td>
</tr>
<tr>
<td>$y$</td>
<td>plant population</td>
<td>m\textsuperscript{2}</td>
<td>[C21]</td>
</tr>
<tr>
<td>$Z_{sC}$</td>
<td>shoot-root C transfer</td>
<td>g C m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C50]</td>
</tr>
<tr>
<td>$Z_{sN,P}$</td>
<td>shoot-root N,P transfer</td>
<td>g N,P m\textsuperscript{2} h\textsuperscript{-1}</td>
<td>[C51]</td>
</tr>
</tbody>
</table>

\(0.6\) Kimmins (2004)

\(0.28 (z = \text{leaf}), 0.24 (z = \text{root and other non-foliary}), 0.20 (z = \text{wood})\) Waring and Running (1998)
<table>
<thead>
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<th>Description</th>
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<td>$Z_{rC}$</td>
<td>root-mycorrhizal C transfer</td>
<td>g C m$^{-2}$ h$^{-1}$</td>
<td>[C52]</td>
</tr>
<tr>
<td>$Z_{rN,P}$</td>
<td>root-mycorrhizal N,P transfer</td>
<td>g N,P m$^{-2}$ h$^{-1}$</td>
<td>[C53]</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>CO$_2$ compensation point in C$_3$ mesophyll</td>
<td>$\mu$M</td>
<td>[C6a,C6c,C7b]</td>
</tr>
<tr>
<td>$\Gamma_{(b4)}$</td>
<td>CO$_2$ compensation point in C$_4$ bundle sheath</td>
<td>$\mu$M</td>
<td>[C44,C45b]</td>
</tr>
<tr>
<td>$\Gamma_{(m4)}$</td>
<td>CO$_2$ compensation point in C$_4$ mesophyll</td>
<td>$\mu$M</td>
<td>[C29,C30b]</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>shape parameter for response of $J$ to $I$</td>
<td>-</td>
<td>[C8a] 0.7</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>shape parameter for response of $J$ to $I$</td>
<td>-</td>
<td>[C31,C46] 0.75</td>
</tr>
<tr>
<td>$\chi$</td>
<td>area:mass ratio of leaf growth</td>
<td>m g$^{-3}$</td>
<td>[C21] 0.0125 Grant and Hesketh (1992)</td>
</tr>
<tr>
<td>$\chi_{C_{4(b4)}}$</td>
<td>non-structural C$_4$ fixation product in C$_4$ bundle sheath</td>
<td>g C m$^{-2}$</td>
<td>[C37,C38,C41]</td>
</tr>
<tr>
<td>$\chi_{C_{4(m4)}}$</td>
<td>non-structural C$_4$ fixation product in C$_4$ mesophyll</td>
<td>g C m$^{-2}$</td>
<td>[C37,C40]</td>
</tr>
<tr>
<td>$[\chi_{C_{3(b4)}}]$</td>
<td>concentration of non-structural C$_3$ fixation product in C$_4$ bundle sheath</td>
<td>g g$^{-1}$</td>
<td>[C49]</td>
</tr>
<tr>
<td>$[\chi_{C_{4(m4)}}]$</td>
<td>concentration of non-structural C$_4$ fixation product in C$_4$ mesophyll</td>
<td>$\mu$M</td>
<td>[C34]</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>quantum yield</td>
<td>$\mu$mol e$^-$ $\mu$mol quanta$^{-1}$</td>
<td>[C8a] 0.45 Farquhar et al. (1980)</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>quantum yield</td>
<td>$\mu$mol e$^-$ $\mu$mol quanta$^{-1}$</td>
<td>[C31,C46] 0.45 Farquhar et al., (1980)</td>
</tr>
<tr>
<td>$\kappa_{C_{4(b4)}}$</td>
<td>conductance to CO$_2$ leakage from C$_4$ bundle sheath</td>
<td>h$^{-1}$</td>
<td>[C39] 20</td>
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<tr>
<td>$\psi_t$</td>
<td>canopy turgor potential</td>
<td>MPa</td>
<td>[C4] 1.25 at $\psi_c = 0$</td>
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Section D: Soil Water, Heat, Gas and Solute Fluxes

Surface Water Flux

\[ Q_{x}(x,y,z) = v_{x}(x,y) \cdot d_{w}(x,y) \cdot L_{x}(x,y) \]
\[ Q_{y}(x,y,z) = v_{y}(x,y) \cdot d_{w}(x,y) \cdot L_{y}(x,y) \]
\[ d_{x,y} = \max(0, d_{w}(x,y) + d_{d}(x,y) - d_{d}(x,y)) \cdot d_{w}(x,y) / (d_{w}(x,y) + d_{d}(x,y)) \]
\[ v_{x}(x,y) = R^{0.67} \cdot s_{x}(x,y)^{0.5} / z_{t}(x,y) \]
\[ v_{y}(x,y) = R^{0.67} \cdot s_{y}(x,y)^{0.5} / z_{t}(x,y) \]
\[ v_{z}(x,y) = R^{0.67} \cdot s_{z}(x,y)^{0.5} / z_{t}(x,y) \]
\[ \Delta(d_{w}(x,y)A_{x,y}) / \Delta t = Q_{x}(x,y,z) - Q_{x+1}(x,y,z) + Q_{x-1}(x,y,z) - Q_{x,y+1}(x,y,z) + P - E_{x,y} - Q_{w}(x,y,z) \]

\[ R = s_{t} d_{m} / [2 (s_{t}^{2} + 1) 0.5] \]
\[ s_{x}(x,y) = 2 \cdot \text{abs}(Z + d_{s} + d_{m})_{x,y} - (Z + d_{s} + d_{m})_{x+y+1,y} / (L_{x}(x,y) + L_{x}(x+1,y)) \]
\[ s_{y}(x,y) = 2 \cdot \text{abs}(Z + d_{s} + d_{m})_{x,y} - (Z + d_{s} + d_{m})_{x,y+1} / (L_{y}(x,y) + L_{y}(x,y+1)) \]
\[ LE_{i} = L (e_{a} - e_{i(T_{a},Q_{i})}) / r_{w} \]
\[ LE_{a} = L (e_{a} - e_{a(T_{a},Q_{a})}) / r_{w} \]

Subsurface Water Flux

\[ Q_{ws}(x,y,z) = K_{x}^{*} (\psi_{xx,y,z} - \psi_{xx+1,y,z}) \]
\[ Q_{ws}(x,y,z) = K_{y}^{*} (\psi_{xx,y,z} - \psi_{xx,y+1,z}) \]

2D Manning equation in \( x \) (EW) and \( y \) (NS) directions

[\text{D1}] surface water depth

[\text{D2}] runoff velocity over E slope

[\text{D3}] runoff velocity over S slope

[\text{D4}] runoff velocity over W slope

[\text{D5}] runoff velocity over N slope

2D kinematic wave theory for overland flow

wetted perimeter

[\text{D5a}] 2D slope from topography and pooled surface water in \( x \) (EW) and \( y \) (NS) directions

evaporation from surface litter

[\text{D5b}] evaporation from soil surface

[\text{D6a}] 3D Richard’s or Green-Ampt equation depending on saturation of source or target cell in \( x \) (EW),

[\text{D7}]
\[ Q_{wz(x,y,z)} = K'_x (\psi_{s(x,y,z)} - \psi_{s(x,y,z+1)}) \]

\[ \Delta \theta_{w(x,y,z)}/\Delta t = (Q_{wx(x,y)} - Q_{wz+1}(x,y)) + Q_{wy(x,y)} - Q_{wz+1}(x,y) + Q_{wz(x,y)} - Q_{wz+1}(x,y) + Q_{z(x,y,z)} / L(z(x,y,z)) \]

\[ K'_x = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

\[ = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

\[ K'_y = 2K_{x,y,z} K_{x+1,y+1,z} / (K_{x,y,z} L_{x+1,y,z} + K_{x+1,y,z} L_{x,y,z}) \]

\[ = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

\[ K'_z = 2K_{x,y,z} / (K_{x,y,z} L_{x,y,z+1} + K_{x,y,z+1} L_{x,y,z}) \]

\[ = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

\[ K'_z = 2K_{x,y,z} K_{y+1,z+1} / (K_{x,y,z} L_{x,y,z+1} + K_{x,y,z+1} L_{x,y,z}) \]

\[ = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

\[ = 2K_{x,y,z} / (L_{x,y,z+1} + L_{x,y,z-1}) \]

**Exchange with Water Table**

\[ Q_{w(x,y,z)} = K_{x,y,z} [\psi' - \psi_{w(x,y,z)} + 0.01 (d_{x,y,z} - d_i)] / (L_{x,y} + 0.5 L_{x,y,z} \text{ or } d_{x,y,z} > d_i) \]

\[ Q_{y(x,y,z)} = K_{x,y,z} [\psi' - \psi_{w(x,y,z)} + 0.01 (d_{x,y,z} - d_i)] / (L_{x,y} + 0.5 L_{x,y,z} \text{ or } d_{x,y,z} > d_i) \]

**Heat Flux**

\[ R_a + LE + H + G = 0 \]

\[ G_{x(x,y,z)} = 2\kappa_{x,y,z}(x+1,y,z) (T_{x+1,y,z} - T_{x,y,z}) / (L_{x,y+1}(x+1,y,z) + L_{x,y-1}(x+1,y,z) + c_u T_{x,y,z} Q_{w(x,y,z)}) \]

\[ G_{y(x,y,z)} = 2\kappa_{x,y,z}(x,y+1,z) (T_{x,y+1,z} - T_{x,y,z}) / (L_{x,y+1}(x,y+1,z) + L_{x,y-1}(x,y+1,z) + c_u T_{x,y,z} Q_{w(x,y,z)}) \]

y (NS) and z (vertical) directions

3D water transfer plus freeze-thaw in direction x if source and destination cells are unsaturated in direction x if source cell is saturated in direction x if destination cell is saturated in direction y if source and destination cells are unsaturated in direction y if source cell is saturated in direction y if destination cell is saturated in direction z if source and destination cells are unsaturated in direction z if source cell is saturated in direction z if destination cell is saturated

if \( \psi_{s(x,y,z)} > \psi' + 0.01(d_{x,y,z} - d_i) \) for all depths \( z \) from \( d_{x,y,z} \) to \( d_i \)

or if \( d_{x,y,z} > d_i \)

for each canopy, snow, residue and soil surface, depending on exposure 3D conductive – convective heat flux among snowpack, surface residue and soil layers in x (EW), y (NS) and z (vertical) directions

[D8]

[D9a]

[D9b]

[D9a]

[D9b]

[D10]

[D11]

[D12a]

[D12b]
\[ G_{(x,y,z)} = 2 \kappa_{(x,y,z)} (T_{(x,y,z)} - T_{(x,y,z+1)}) / (L_z (x,y,z) + L_z (x,y,z+1)) + c_v T_{(x,y,z)} Q_w z (x,y,z) \]

\[ G_{X (y+1,z)} - G_{X (y,z)} = G_{Y (x+1,z)} - G_{Y (x,z)} + G_{Z (x,y,z)} - G_{Z (x,y,z+1)} + LQ_{f (x,y,z)} + c_w (x,y,z) (T_{(x,y,z)} - T_{(x,y,z)}) / \Delta t = 0 \]

**Gas Flux**

\[ Q_{v p x,y,z} = a_{v p x,y,z} D_{v p} (S^p f_{v p x,y,z} [\gamma_{p x,y,z}] - [\gamma_{p x,y,z}]) \]
\[ Q_{g x,y,z} = a_{gx,y,z} D_{g} (S^g f_{g x,y,z} [\gamma_{g x,y,z}] - [\gamma_{g x,y,z}]) \]
\[ Q_{g p x,y,z} = 8 a_{g x,y,z} [\gamma_{g x,y,z}] / [2 (\gamma_{g x,y,z}) / L_{g x,y,z} + g_{s x,y} (\gamma_{g x,y,z})] / [2 \cdot D_{g p x,y,z} / L_{g x,y,z} + g_{s x,y}] \]
\[ Q_{v p x,y,z} = a_{v p x,y,z} / D_{v p} (S^p f_{v p x,y,z} (\gamma_{p x,y,z}) - \gamma_{p x,y,z}) \]
\[ Q_{g x,y,z} = 8 a_{g x,y,z} / D_{g} (S^g f_{g x,y,z} (\gamma_{g x,y,z}) - \gamma_{g x,y,z}) \]
\[ Q_{g p x,y,z} = b_{g p x,y,z} (\gamma_{g x,y,z}) / D_{g p x,y,z} (\gamma_{g x,y,z}) - \gamma_{g x,y,z}) \]
\[ Q_{g x,y,z} = D_{g x,y,z} (\gamma_{g x,y,z}) / \Sigma_{x,y} \]
\[ D_{g p x,y,z} = D_{g p x,y,z} (\gamma_{p x,y,z}) / \Sigma_{x,y} \]
\[ D_{g x,y,z} = D_{g x,y,z} (\gamma_{g x,y,z}) / \Sigma_{x,y} \]
\[ D_{g p x,y,z} = D_{g p x,y,z} (\gamma_{p x,y,z}) / \Sigma_{x,y} \]

(NS) and z (vertical) directions

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

volatilization – dissolution between aqueous and gaseous phases in soil and root

volatilization – dissolution between gaseous and aqueous phases at the soil surface (z = 1) and the atmosphere

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

convective - conductive gas flux between roots and the atmosphere
gasous diffusivity as a function of air-filled porosity in soil

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

[D12c]
[D13]
[D14a]
[D14b]
[D15a]
[D15b]
[D16a]
[D16b]
[D16c]
[D16d]
[D17a]
[D17b]
[D17c]
[D17d]
Solute Flux

\[ Q_{wx(x,y,z)} = - Q_{wx(x,y,z)} \left[ \gamma_a \kappa_{x,y,z} + 2 D_{synchronous} \left( \left| \gamma_a \right| - \left| \gamma_a + \phi \right| \right) / \left( L_{x(y,z)} + L_{x(y,z)+1} \right) \right] \]

\[ Q_{wy(x,y,z)} = - Q_{wy(x,y,z)} \left[ \gamma_a \kappa_{x,y,z} + 2 D_{synchronous} \left( \left| \gamma_a \right| - \left| \gamma_a + \phi \right| \right) / \left( L_{y(x,z)} + L_{y(x,z)+1} \right) \right] \]

\[ Q_{xz(x,y,z)} = - Q_{xz(x,y,z)} \left[ \gamma_a \kappa_{x,y,z} + 2 D_{synchronous} \left( \left| \gamma_a \right| - \left| \gamma_a + \phi \right| \right) / \left( L_{z(x,y)} + L_{z(x,y)+1} \right) \right] \]

\[ Q_{r(x,y,z)} = - Q_{w(x,y,z)} \left[ \gamma_a \kappa_{x,y,z} + 2 \pi L_{r(x,y,z)} D_{synchronous} \left( \left| \gamma_a \right| - \left| \gamma_a + \phi \right| \right) \ln \left( \left( r_x + r_{r(x,y,z)} \right) / r_{r(x,y,z)} \right) \right] \]

\[ D_{sx(x,y,z)} = D_{sx(x,y,z)} \left| Q_{sx(x,y,z)} \right| + D_{sx(x,y,z)} \left( 0.5 \left( \theta_{sx,y,z} + \theta_{sx+1,y,z} \right) \right) \tau \]

\[ D_{sy(x,y,z)} = D_{sy(x,y,z)} \left| Q_{sy(x,y,z)} \right| + D_{sy(x,y,z)} \left( 0.5 \left( \theta_{sx,y,z} + \theta_{sx+1,y,z} \right) \right) \tau \]

\[ D_{sz(x,y,z)} = D_{sz(x,y,z)} \left| Q_{sz(x,y,z)} \right| + D_{sz(x,y,z)} \left( 0.5 \left( \theta_{sx,y,z} + \theta_{sx+1,y,z} \right) \right) \tau \]

\[ D_{r(x,y,z)} = D_{r(x,y,z)} \left| Q_{r(x,y,z)} \right| + D_{r(x,y,z)} \left( 0.5 \left( \theta_{sx,y,z} + \theta_{sx+1,y,z} \right) \right) \tau \]

\[ D_{x(x,y,z)} = 0.5 \alpha ( L_x (x,y,z) + L_{x(y,z)+1} )^\beta \]

\[ D_{y(x,y,z)} = 0.5 \alpha ( L_y (x,y,z) + L_{y(x,z)+1} )^\beta \]

\[ D_{z(x,y,z)} = 0.5 \alpha ( L_z (x,y,z) + L_{z(x,y)+1} )^\beta \]

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

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

convective - dispersive solute flux between soil and root aqueous phases

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

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

dispersivity as a function of water flow length
## Definition of Variables in Section D

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<thead>
<tr>
<th>Variable</th>
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<th>Equation</th>
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<td>$x$</td>
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<tr>
<td>$y$</td>
<td>grid cell position in north to south direction</td>
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<tr>
<td>$z$</td>
<td>grid cell position in vertical direction</td>
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**subscripts**

<table>
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<th>Reference</th>
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</thead>
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<tr>
<td>$z = 0$: surface residue, $z = 1$ to $n$: soil layers</td>
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</table>

**variables**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
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<th>Equation</th>
<th>Value</th>
<th>Reference</th>
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<td>$A$</td>
<td>area of landscape position</td>
<td>m$^2$</td>
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<tr>
<td>$A_r$</td>
<td>root cross-sectional area of landscape position</td>
<td>m$^2$</td>
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<tr>
<td>$a_{gr}$</td>
<td>air-water interfacial area in roots</td>
<td>m$^2$ m$^{-2}$</td>
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</tr>
<tr>
<td>$a_{gs}$</td>
<td>air-water interfacial area in soil</td>
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<td>[D14a,D15b]</td>
<td>Skopp (1985)</td>
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<td>$\alpha$</td>
<td>dependence of $D_q$ on $L$</td>
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<td>MJ m$^{-2}$ °C$^{-1}$</td>
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<tr>
<td>$c_w$</td>
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<tr>
<td>$D_{dy}$</td>
<td>volatilization - dissolution transfer coefficient for gas $\gamma$</td>
<td>m$^2$ h$^{-1}$</td>
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<td>$D_{gr}$</td>
<td>gaseous diffusivity of gas $\gamma$ in roots</td>
<td>m$^2$ h$^{-1}$</td>
<td>[D16d,D17d]</td>
<td>Luxmoore et al. (1970a,b)</td>
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<tr>
<td>$D_{gs}$</td>
<td>gaseous diffusivity of gas $\gamma$ in soil</td>
<td>m$^2$ h$^{-1}$</td>
<td>[D15a,D16a,b,c,D \ 17a,b,c]</td>
<td>Millington and Quirk (1960)</td>
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<tr>
<td>$D_{g'}$</td>
<td>diffusivity of gas $\gamma$ in air at 0 °C</td>
<td>m$^2$ h$^{-1}$</td>
<td>[D17]</td>
<td>6.43 x 10$^{-2}$ for $\gamma = O_2$</td>
<td>Campbell (1985)</td>
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<tr>
<td>Symbol</td>
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<td>Unit</td>
<td>Reference</td>
<td>Value</td>
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<tr>
<td>( D'_{qr} )</td>
<td>dispersivity in roots</td>
<td>m</td>
<td>[D20d]</td>
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<tr>
<td>( D_q )</td>
<td>dispersivity in soil</td>
<td>m</td>
<td>[D20,D21]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( D_{r1} )</td>
<td>aqueous diffusivity of gas or solute ( \gamma ) in roots</td>
<td>m(^2)h(^{-1})</td>
<td>[D19d,D20d]</td>
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</tr>
<tr>
<td>( D_{r2} )</td>
<td>aqueous diffusivity of gas or solute ( \gamma ) in soil</td>
<td>m(^2)h(^{-1})</td>
<td>[D19,D20]</td>
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<tr>
<td>( D'_{sf} )</td>
<td>diffusivity of gas ( \gamma ) in water at 0 °C</td>
<td>m(^2)h(^{-1})</td>
<td>[D20]</td>
<td>8.57 x 10(^{-6}) for ( \gamma = \text{O}_2 ) Campbell (1985)</td>
<td></td>
</tr>
<tr>
<td>( d_m )</td>
<td>depth of mobile surface water</td>
<td>m</td>
<td>[D1,D2,D5a,D6]</td>
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<tr>
<td>( d_i )</td>
<td>depth of surface ice</td>
<td>m</td>
<td>[D2]</td>
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<tr>
<td>( d_s )</td>
<td>maximum depth of surface water storage</td>
<td>m</td>
<td>[D2,D5b]</td>
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<tr>
<td>( d_t )</td>
<td>depth of external water table</td>
<td>m</td>
<td>[D10]</td>
<td></td>
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</tr>
<tr>
<td>( d_w )</td>
<td>depth of surface water</td>
<td>m</td>
<td>[D1,D2]</td>
<td></td>
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</tr>
<tr>
<td>( d_z )</td>
<td>depth to mid-point of soil layer</td>
<td>m</td>
<td>[D10]</td>
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<tr>
<td>( E )</td>
<td>evaporation or transpiration flux</td>
<td>m(^3)m(^{-2})h(^{-1})</td>
<td>[D4,D11]</td>
<td></td>
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<tr>
<td>( e_a )</td>
<td>atmospheric vapor density</td>
<td>m(^3)m(^{-3})</td>
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<tr>
<td>( e_{(T_l,\psi_l)} )</td>
<td>surface litter vapor density at current ( T_l ) and ( \psi_l )</td>
<td>g m(^{-3})</td>
<td>[D6a]</td>
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<td>( e_{(T_s,\psi_s)} )</td>
<td>soil surface vapor density at current ( T_s ) and ( \psi_s )</td>
<td>g m(^{-3})</td>
<td>[D6b]</td>
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<tr>
<td>( f_{k_{\gamma}} )</td>
<td>temperature dependence of ( S'_{\gamma} )</td>
<td>-</td>
<td>[D14,D15b,D18]</td>
<td>Wilhelm et al. (1977)</td>
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<tr>
<td>( f_{k_g} )</td>
<td>temperature dependence of ( D'_{gf} )</td>
<td>-</td>
<td>[D17]</td>
<td>Campbell (1985)</td>
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<tr>
<td>( f_{k_s} )</td>
<td>temperature dependence of ( D'_{sf} )</td>
<td>-</td>
<td>[D20]</td>
<td>Campbell (1985)</td>
<td></td>
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<tr>
<td>( G )</td>
<td>soil surface heat flux</td>
<td>m(^3)m(^{-2})h(^{-1})</td>
<td>[D11]</td>
<td></td>
<td></td>
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</table>
\( G_x, G_y, G_z \) soil heat flux in \( x, y \) or \( z \) directions  
\( g_a \) boundary layer conductance  
\( \gamma \) gas (\( \text{H}_2\text{O}, \text{CO}_2, \text{O}_2, \text{CH}_4, \text{NH}_3, \text{N}_2\text{O}, \text{N}_2, \text{H}_2 \)) or solute (from Section E)  
\([\gamma_a]\) atmospheric concentration of gas \( \gamma \)  
\([\gamma_{gr}]\) gasous concentration of gas \( \gamma \) in roots  
\([\gamma_{gs}]\) gasous concentration of gas \( \gamma \) in soil  
\([\gamma_{sr}]\) aqueous concentration of gas \( \gamma \) in roots  
\([\gamma_{sr}]\) aqueous concentration of gas \( \gamma \) at root surface  
\([\gamma_{ss}]\) aqueous concentration of gas \( \gamma \) in soil  
\( H \) sensible heat flux  
\( K \) hydraulic conductivity  
\( K', K_y, K_z \) hydraulic conductance in \( x, y \) or \( z \) directions  
\( \kappa \) thermal conductivity  
\( L_i \) root length  
\( L_e \) distance from boundary to external water table in \( x \) or \( y \) directions  
\( L_x, L_y, L_z \) length of landscape element in \( x, y \) or \( z \) directions  
\( LE_i \) latent heat flux from surface litter  
\( LE_s \) latent heat flux from soil surface
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$L$</td>
<td>latent heat of evaporation</td>
<td>MJ m$^{-3}$</td>
<td>[D6,D11,D13] 2460</td>
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<tr>
<td>$M_f$</td>
<td>atomic mass of gas $\gamma$</td>
<td>g mol$^{-1}$</td>
<td>[D18]</td>
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<td>$P$</td>
<td>precipitation flux</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
<td>[D4]</td>
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<tr>
<td>$Q_{byc}$</td>
<td>bubbling flux</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[D18]</td>
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<td>$Q_{drl}$</td>
<td>volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in roots</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[D14b]</td>
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<tr>
<td>$Q_{dso}$</td>
<td>volatilization – dissolution of gas $\gamma$ between aqueous and gaseous phases in soil</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[D14a,D15b]</td>
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<tr>
<td>$Q_f$</td>
<td>freeze-thaw flux (thaw +ve)</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
<td>[D8,D13]</td>
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<td>$Q_{gry}$</td>
<td>gaseous flux of gas $\gamma$ between roots and the atmosphere</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[D16d]</td>
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<td>$Q_{gyr}$</td>
<td>gaseous flux of gas $\gamma$ in soil</td>
<td>g m$^{-2}$ h$^{-1}$</td>
<td>[D15a,D16a,b,c]</td>
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<td>$Q_{rx}$, $Q_{ry}$</td>
<td>surface water flow in $x$ or $y$ directions</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
<td>[D1,D4]</td>
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<td>$Q_{ry}$</td>
<td>aqueous flux of gas or solute $\gamma$ in soil</td>
<td>g m$^{-2}$ h$^{-1}$</td>
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<td>$Q_{rij}$</td>
<td>aqueous flux of gas or solute $\gamma$ from soil and root aqueous phases to root surface</td>
<td>g m$^{-2}$ h$^{-1}$</td>
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<td>$Q_t$</td>
<td>water flux between boundary grid cell and external water table in $x$ or $y$ directions</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
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<tr>
<td>$Q_{wr}$</td>
<td>root water uptake</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
<td>[D19d, D20d]</td>
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<tr>
<td>$Q_{wx}$, $Q_{wy}$, $Q_{wz}$</td>
<td>subsurface water flow in $x$, $y$ or $z$ directions</td>
<td>m$^3$ m$^{-2}$ h$^{-1}$</td>
<td>[D4,D7,D8,D12,D16,D19,D20]</td>
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<tr>
<td>$\theta_g$</td>
<td>air-filled porosity</td>
<td>m$^3$ m$^{-3}$</td>
<td>[D17a,b,c]</td>
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<td>$\theta_{pr}$</td>
<td>root porosity</td>
<td>m$^3$ m$^{-3}$</td>
<td>[D17d] dryland spp. 0.10 wetland spp. 0.20 Luxmoore et al. (1970a,b)</td>
</tr>
<tr>
<td>$\theta_{ps}$</td>
<td>soil porosity</td>
<td>m$^3$ m$^{-3}$</td>
<td>[D17a,b,c]</td>
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<td>$\theta_w$</td>
<td>water-filled porosity</td>
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<td>$R$</td>
<td>ratio of cross-sectional area to perimeter of surface flow</td>
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<td>net radiation</td>
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<td>$r_{al}$</td>
<td>surface litter boundary layer resistance</td>
<td>m h$^{-1}$</td>
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<td>$r_{as}$</td>
<td>Soil surface boundary layer resistance</td>
<td>m h$^{-1}$</td>
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<td>$r_{qi.r}$</td>
<td>radius of root or mycorrhizal aerenchyma</td>
<td>m</td>
<td>[D19d]</td>
</tr>
<tr>
<td>$r_{ri,r}$</td>
<td>root or mycorrhizal radius</td>
<td>m</td>
<td>[D19d]</td>
</tr>
<tr>
<td>$r_s$</td>
<td>thickness of soil water films</td>
<td>m</td>
<td>[D19d, D21d]</td>
</tr>
<tr>
<td>$S'_\gamma$</td>
<td>Ostwald solubility coefficient of gas $\gamma$ at 30°C</td>
<td>-</td>
<td>[D14,D15b,D18]</td>
</tr>
<tr>
<td>$s_r$</td>
<td>slope of channel sides during surface flow</td>
<td>m m$^{-1}$</td>
<td>[D5a]</td>
</tr>
<tr>
<td>$s_x$, $s_y$</td>
<td>slope in $x$ or $y$ directions</td>
<td>m m$^{-1}$</td>
<td>[D3,D5b]</td>
</tr>
<tr>
<td>$T$</td>
<td>soil temperature</td>
<td>°C</td>
<td>[D12,D18]</td>
</tr>
<tr>
<td>$\tau$</td>
<td>tortuosity</td>
<td>-</td>
<td>[D20]</td>
</tr>
<tr>
<td>$v_x$, $v_y$</td>
<td>velocity of surface flow in $x$ or $y$ directions</td>
<td>m h$^{-1}$</td>
<td>[D1,D3]</td>
</tr>
<tr>
<td>$\psi'$</td>
<td>soil water potential at saturation</td>
<td>MPa</td>
<td>[D10]</td>
</tr>
<tr>
<td>$\psi_s$</td>
<td>soil water potential</td>
<td>MPa</td>
<td>[D7,D10]</td>
</tr>
<tr>
<td>$Z$</td>
<td>surface elevation</td>
<td>m</td>
<td>[D5b]</td>
</tr>
<tr>
<td>$z_r$</td>
<td>Manning's roughness coefficient</td>
<td>m$^{-1/3}$ h</td>
<td>[D3]</td>
</tr>
</tbody>
</table>

Wilhelm et al. (1977): $0.0293$ for $\gamma = O_2$, $5.0 \times 10^{-3}$
Section E: Solute Transformations

Precipitation - Dissolution Equilibria

\[
\text{Al(OH)}_3(s) \rightleftharpoons (\text{Al}^{3+}) + 3(\text{OH}^-) \quad \text{(amorphous Al(OH)}_3) \quad [-33.0 \text{ [E1]}^1
\]

\[
\text{Fe(OH)}_3(s) \rightleftharpoons (\text{Fe}^{3+}) + 3(\text{OH}^-) \quad \text{(soil Fe)} \quad [-39.3 \text{ [E2]}
\]

\[
\text{CaCO}_3(s) \rightleftharpoons (\text{Ca}^{2+}) + (\text{CO}_3^{2-}) \quad \text{(calcite)} \quad [-9.28 \text{ [E3]}
\]

\[
\text{CaSO}_4(s) \rightleftharpoons (\text{Ca}^{2+}) + (\text{SO}_4^{2-}) \quad \text{(gypsum)} \quad [-4.64 \text{ [E4]}
\]

\[
\text{AlPO}_4(s) \rightleftharpoons (\text{Al}^{3+}) + (\text{PO}_4^{3-}) \quad \text{(variscite)} \quad [-22.1 \text{ [E5]}^2
\]

\[
\text{FePO}_4(s) \rightleftharpoons (\text{Fe}^{3+}) + (\text{PO}_4^{3-}) \quad \text{(strengite)} \quad [-26.4 \text{ [E6]}
\]

\[
\text{CaH}_2\text{PO}_4(s) \rightleftharpoons (\text{Ca}^{2+}) + 2(\text{H}_2\text{PO}_4^-) \quad \text{(monocalcium phosphate)} \quad [-1.15 \text{ [E7]}^3
\]

\[
\text{CaHPO}_4(s) \rightleftharpoons (\text{Ca}^{2+}) + (\text{HPO}_4^{2-}) \quad \text{(monetite)} \quad [-6.92 \text{ [E8]}
\]

\[
\text{Ca}_5(\text{PO}_4)_3\text{OH}(s) \rightleftharpoons 5(\text{Ca}^{2+}) + 3(\text{PO}_4^{3-}) + (\text{OH}^-) \quad \text{(hydroxyapatite)} \quad [-58.2 \text{ [E9]}
\]

Cation Exchange Equilibria

\[
\text{X-Ca} + 2(\text{NH}_4^+) \rightleftharpoons 2\text{X-NH}_4 + (\text{Ca}^{2+}) \quad 1.00 \text{ [E10]}
\]

\[
3\text{X-Ca} + 2(\text{Al}^{3+}) \rightleftharpoons 2\text{X-Al} + 3(\text{Ca}^{2+}) \quad 1.00 \text{ [E11]}
\]

\[
\text{X-Ca} + (\text{Mg}^{2+}) \rightleftharpoons \text{X-Mg} + (\text{Ca}^{2+}) \quad 0.60 \text{ [E12]}
\]

\[
\text{X-Ca} + 2(\text{Na}^+) \rightleftharpoons 2\text{X-Na} + (\text{Ca}^{2+}) \quad 0.16 \text{ [E13]}
\]

\[
\text{X-Ca} + 2(\text{K}^+) \rightleftharpoons 2\text{X-K} + (\text{Ca}^{2+}) \quad 3.00 \text{ [E14]}
\]

\[
\text{X-Ca} + 2(\text{H}^+) \rightleftharpoons 2\text{X-H} + (\text{Ca}^{2+}) \quad 1.00 \text{ [E15]}
\]

---

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

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

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

4 $X$- denotes surface exchange site for cation or anion adsorption.
3 X-Al + 2 (X-Ca + X-Mg) + X-NH₄ + X-K + X-Na + X-H = CEC  \[E16\]

**Anion Adsorption Equilibria**

\[ X-\text{OH}_2^+ \rightleftharpoons X-\text{OH} + (H^+) \] \[-7.35 \quad [E17]\]

\[ X-\text{OH} \rightleftharpoons X-\text{O}^- + (H^+) \] \[-8.95 \quad [E18]\]

\[ X-\text{H}_2\text{PO}_4^- + \text{H}_2\text{O} \rightleftharpoons X-\text{OH}_2^+ + (\text{H}_2\text{PO}_4^-) \] \[-2.80 \quad [E19]\]

\[ X-\text{H}_2\text{PO}_4^- + \text{OH}^- \rightleftharpoons X-\text{OH} + (\text{H}_2\text{PO}_4^-) \] \[4.20 \quad [E20]\]

\[ X-\text{HPO}_4^2^- + \text{OH}^- \rightleftharpoons X-\text{OH} + (\text{HPO}_4^{2-}) \] \[2.60 \quad [E21]\]

\[ X-\text{OH}_2^+ + X-\text{OH} + X-\text{O}^- + X-\text{H}_2\text{PO}_4^- + X-\text{HPO}_4^2^- + X-\text{COO}^- = \text{AEC} \]

**Organic Acid Equilibria**

\[ X-\text{COOH} \rightleftharpoons X-\text{COO}^- + (H^+) \] \[-5.00 \quad [E23]\]

**Ion Pair Equilibria**

\[(\text{NH}_4^+) \rightleftharpoons (\text{NH}_3) + (H^+) \] \[-9.24 \quad [E24]\]

\[ \text{H}_2\text{O} \rightleftharpoons (H^+) + (\text{OH}^-) \] \[-14.3 \quad [E25]\]

\[(\text{CO}_2)_{(g)} + \text{H}_2\text{O} \rightleftharpoons (H^+) + (\text{HCO}_3^-) \] \[-6.42 \quad [E26]\]

\[(\text{HCO}_3^-) \rightleftharpoons (H^+) + (\text{CO}_3^{2-}) \] \[-10.4 \quad [E27]\]

\[(\text{AlOH}^{2+}) \rightleftharpoons (\text{Al}^{3+}) + (\text{OH}^-) \] \[-9.06 \quad [E28]\]

\[(\text{Al(OH)}_2^+) \rightleftharpoons (\text{AlOH}^{2+}) + (\text{OH}^-) \] \[-10.7 \quad [E29]\]

\[(\text{Al(OH)}_3^-) \rightleftharpoons (\text{Al(OH)}_2^+) + (\text{OH}^-) \] \[-5.70 \quad [E30]\]

\[(\text{Al(OH)}_4^-) \rightleftharpoons (\text{Al(OH)}_3^-) + (\text{OH}^-) \] \[-5.10 \quad [E31]\]

\[(\text{Al(OH)}_5^-) \rightleftharpoons (\text{Al(OH)}_4^-) + (\text{OH}^-) \] \[-3.80 \quad [E32]\]

\[(\text{FeOH}^{2+}) \rightleftharpoons (\text{Fe}^{3+}) + (\text{OH}^-) \] \[-12.1 \quad [E33]\]

\[(\text{Fe(OH)}_2^+) \rightleftharpoons (\text{Fe(OH)}^{2+}) + (\text{OH}^-) \] \[-10.8 \quad [E34]\]

\[(\text{Fe(OH)}_3^-) \rightleftharpoons (\text{Fe(OH)}_2^+) + (\text{OH}^-) \] \[-6.94 \quad [E35]\]

\[(\text{Fe(OH)}_4^-) \rightleftharpoons (\text{Fe(OH)}_3^-) + (\text{OH}^-) \] \[-5.84 \quad [E36]\]
\[
\begin{align*}
(\text{FeSO}_4) & \rightleftharpoons (\text{Fe}^{3+}) + (\text{SO}_4^{2-}) & -4.15 & \text{[E37]} \\
(\text{CaOH}^+) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{OH}^-) & -1.90 & \text{[E38]} \\
(\text{CaCO}_3) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{CO}_3^{2-}) & -4.38 & \text{[E39]} \\
(\text{CaHCO}_3^+) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{HCO}_3^-) & -1.87 & \text{[E40]} \\
(\text{CaSO}_4) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{SO}_4^{2-}) & -2.92 & \text{[E41]} \\
(\text{MgOH}^+) & \rightleftharpoons (\text{Mg}^{2+}) + (\text{OH}^-) & -3.15 & \text{[E42]} \\
(\text{MgCO}_3) & \rightleftharpoons (\text{Mg}^{2+}) + (\text{CO}_3^{2-}) & -3.52 & \text{[E43]} \\
(\text{MgHCO}_3^+) & \rightleftharpoons (\text{Mg}^{2+}) + (\text{HCO}_3^-) & -1.17 & \text{[E44]} \\
(\text{MgSO}_4) & \rightleftharpoons (\text{Mg}^{2+}) + (\text{SO}_4^{2-}) & -2.68 & \text{[E45]} \\
(\text{NaCO}_3) & \rightleftharpoons (\text{Na}^+) + (\text{CO}_3^{2-}) & -3.35 & \text{[E46]} \\
(\text{NaSO}_4) & \rightleftharpoons (\text{Na}^+) + (\text{SO}_4^{2-}) & -0.48 & \text{[E47]} \\
(\text{KSO}_4) & \rightleftharpoons (\text{K}^+) + (\text{SO}_4^{2-}) & -1.30 & \text{[E48]} \\
(\text{H}_3\text{PO}_4) & \rightleftharpoons (\text{H}^+) + (\text{H}_2\text{PO}_4^-) & -2.15 & \text{[E49]} \\
(\text{H}_2\text{PO}_4^-) & \rightleftharpoons (\text{H}^+) + (\text{HPO}_4^{2-}) & -7.20 & \text{[E50]} \\
(\text{HPO}_4^{2-}) & \rightleftharpoons (\text{H}^+) + (\text{PO}_4^{3-}) & -12.4 & \text{[E51]} \\
(\text{FeH}_2\text{PO}_4^{2-}) & \rightleftharpoons (\text{Fe}^{3+}) + (\text{H}_2\text{PO}_4^-) & -5.43 & \text{[E52]} \\
(\text{FeHPO}_4^+) & \rightleftharpoons (\text{Fe}^{3+}) + (\text{HPO}_4^{2-}) & -10.9 & \text{[E53]} \\
(\text{CaH}_2\text{PO}_4^+) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{H}_2\text{PO}_4^-) & -1.40 & \text{[E54]} \\
(\text{CaHPO}_4) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{HPO}_4^{2-}) & -2.74 & \text{[E55]} \\
(\text{CaPO}_4) & \rightleftharpoons (\text{Ca}^{2+}) + (\text{PO}_4^{3-}) & -6.46 & \text{[E56]} \\
(\text{MgHPO}_4) & \rightleftharpoons (\text{Mg}^{2+}) + (\text{HPO}_4^{2-}) & -2.91 & \text{[E57]}
\end{align*}
\]
Section H: Inorganic N Transformations

Mineralization and Immobilization of Ammonium by All Microbial Populations

\[ I_{NH_4,l,n,j} = (M_{l,m,j,c} C_{N_j} - M_{l,m,j,N}) \]  \[ (I_{NH_4,l,n,j} < 0) \]  \[ [H1a] \]

\[ I_{NH_4,l,n,j} = (M_{l,m,j,c} C_{N_j} - M_{l,m,j,N}) [NH_3'^+] / ([NH_3'^+] + K_{NH_3}) \]  \[ (I_{NH_4,l,n,j} > 0) \]  \[ [H1b] \]

\[ I_{NO_3,l,n,j} = (M_{l,m,j,c} C_{N_j} - (M_{l,m,j,N} + I_{NH_4,l,n})) [NO_3^-] / ([NO_3^-] + K_{NO_3}) \]  \[ (I_{NO_3,l,n,j} > 0) \]  \[ [H1b] \]

Oxidation of DOC and Reduction of Oxygen by Heterotrophs

\[ X_{DOC,l,h} = \{X_{DOC} - M_{l,h,a} [DOC] / ([DOC]) + K_{S,h}\} f_i \]  \[ [H2] \]

\[ R'_{O_2,l,h} = R'_{O_2,l,h} \]  \[ [H3] \]

\[ R_{O_2,l,h} = 4\pi n M_{l,h,a} D_{O_2} ([O_2] - [O_{2m,l,h}]) (r_m r_w / (r_w - r_m)) \]

\[ = R'_{O_2,l,h} [O_{2m,l,h}] / ([O_{2m,l,h}] + K_{O_{2h}}) \]  \[ [H4a] \]

\[ X_{DOC,l,h} = X_{DOC,l,h} \]  \[ [H5] \]

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

\[ R'_{NO_3,l,d} = E_{NO_3} (R'_{O_2,l,d} - R_{O_2,l,d})(1.0 + K_t (R'_{O_2,l,d} - R_{O_2,l,d}) / V_i) \]  \[ [H6] \]

\[ R_{NO_3,l,d} = R'_{NO_3,l,d} [NO_3^-] / ([NO_3^-] + K_{NO_3})(1.0 + ([NO_2^-] K_{NO_2} / ([NO_2^-] K_{NO_2}))) \]  \[ [H7] \]

\[ R_{NO_2,l,d} = R_{NO_3,l,d} - R_{NO_2,l,d} [NO_2^-] / ([NO_2^-] + K_{NO_2})(1.0 + ([O_2] K_{NO_2} / ([O_2] K_{NO_2}))) \]  \[ [H8] \]

\[ X_{DOC,l,d} = X_{DOC,l,d} \]  \[ [H9] \]

Oxidation of Ammonia and Reduction of Oxygen by Nitrifiers

\[ X_{NH_3,l,a} = X_{NH_3} M_{l,a,n} \]  \[ [NH_3S] / ([NH_3S] + K_{NH_3}) \]  \[ [CO_2S] / ([CO_2S] + K_{CO_2}) \]  \[ f_i \]  \[ [H11] \]

\[ R_{O_2,l,a} = R'_{NH_3} X_{NH_3,l,a} + R'_{QC} X_{C_1,a} \]  \[ [H12] \]

\[ R_{O_2,l,a} = 4\pi n M_{l,a,n} D_{O_2} ([O_2] - [O_{2m,l,a}]) (r_m r_w / (r_w - r_m)) \]

\[ = R'_{O_2,l,a} [O_{2m,l,a}] / ([O_{2m,l,a}] + K_{O_{2h}}) \]  \[ [H13a] \]

\[ X_{NH_3,l,a} = X_{NH_3,l,a} R_{O_2,l,a} / R_{O_2,l,a} \]  \[ [H14] \]

Oxidation of Nitrite and Reduction of Oxygen by Nitrifiers

\[ X_{NO_2,l,o} = X_{NO_2} M_{l,o,a} \]  \[ [NO_2^-] / ([NO_2^-] + K_{NO_2}) \]  \[ [CO_2S] / ([CO_2S] + K_{CO_2}) \]  \[ f_i \]  \[ [H15] \]

\[ R_{O_2,l,o} = R'_{NO_2} X_{NO_2,l,o} + R'_{QC} X_{C_1,o} \]  \[ [H16] \]
\[ R_{O_2,i,o} = 4\pi n M_{i,0,a} D_{O_2} (r_m r_w / (r_w - r_m)) \left( [O_{2a}] - [O_{2m,o}] \right) \]
\[ = R'_{O_2,i,o} [O_{2m,i,o}] / ([O_{2m,i,o}] + K_{O_{2w}}) \]
\[ X_{NO_2,i,o} = X'_{NO_2,i,o} R_{O_2,i,o} / R_{O_2,i,o} \]

**Oxidation of Ammonia and Reduction of Nitrite by Nitrifiers**

\[ R'_{NO_2,i,n} = E_{NO} (R'_{O_2,i,n} - R_{O_2,i,n})/(1.0 + K_e (R'_{O_2,i,n} - R_{O_2,i,n})/V_i) \]
\[ R_{NO_2,i,n} = R'_{NO_2,i,n} \{ [NO_2] / ([NO_2] + K_{NO_2}) \} \{ [CO_2] / ([CO_2] + K_{CO_2}) \} \]
\[ X_{NH_3,i,n} = X_{NH_3,i,n} (from [H14]) + 0.33 R_{NO_2,i,n} \]

---

### Definition of Variables in Section H

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Units</th>
<th>Equations</th>
<th>Input Values</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>active component of (M_{i,m})</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(d)</td>
<td>heterotrophic denitrifier population (subset of (h))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(h)</td>
<td>heterotrophic community (subset of (m))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(i)</td>
<td>substrate-microbe complex</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(j)</td>
<td>kinetic components of (M_{i,m})</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(m)</td>
<td>all microbial communities</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(n)</td>
<td>autotrophic ammonia oxidizer population (subset of (m))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(o)</td>
<td>autotrophic nitrite oxidizer population (subset of (m))</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**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**

- \(C_{Nj}\): maximum ratio of \(M_{i,m,j,N}\) to \(M_{i,m,j,C}\) maintained by \(M_{i,m,j}\)
- \([CO_2]\): \(CO_2\) concentration in soil solution
- \([DOC]\): concentration of dissolved decomposition products
- \(D_{O_2}\): aqueous dispersivity-diffusivity of \(O_2\)
- \(E_{NOx}\): \(\epsilon\) accepted by \(NO_x\) vs. \(O_2\) when oxidizing \(DOC\)

\(28/32 = 0.875\)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$F_{\text{NO}_x}$</td>
<td>$e^{-}$ donated by C vs. $e^{-}$ accepted by NO$_x$ when oxidizing DOC</td>
<td>g e g N$^{-1}$</td>
<td>[H10]</td>
</tr>
<tr>
<td>$F_{\text{N}_2\text{O}}$</td>
<td>$e^{-}$ donated by C vs. $e^{-}$ accepted by N$_2$O when oxidizing DOC</td>
<td>g e g N$^{-1}$</td>
<td>[H10]</td>
</tr>
<tr>
<td>$f_{i}$</td>
<td>temperature function for microbial processes</td>
<td>-</td>
<td>[H2,H11,H15]</td>
</tr>
<tr>
<td>$I_{\text{NH}_4^{+},C}$</td>
<td>mineralization ($I_{\text{NH}<em>4^{+},C} &lt; 0$) or immobilization ($I</em>{\text{NH}_4^{+},C} &gt; 0$) of NH$<em>4^{+}$ by M$</em>{i,n,C}$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H1]</td>
</tr>
<tr>
<td>$I_{\text{NO}_3^{-},C}$</td>
<td>immobilization ($I_{\text{NO}_3^{-},C} &gt; 0$) of NO$<em>3^{-}$ by M$</em>{i,n,C}$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H1]</td>
</tr>
<tr>
<td>$K_{\text{CO}_2}$</td>
<td>Michaelis-Menten constant for reduction of CO$<em>2$S by M$</em>{i,n,a}$ and M$_{i,o,a}$</td>
<td>g C m$^{-3}$</td>
<td>[H11,H15,H20]</td>
</tr>
<tr>
<td>$K_{\text{NH}_4^{+}}$</td>
<td>M-M constant for oxidation of NH$_3$S by nitrifiers</td>
<td>g N m$^{-3}$</td>
<td>0.0002</td>
</tr>
<tr>
<td>$K_e$</td>
<td>inhibition constant for electrons not accepted by O$_2$ and transferred to N oxides</td>
<td>-</td>
<td>0.5</td>
</tr>
<tr>
<td>$K_{\text{NH}_4^{+}}$</td>
<td>M-M constant for microbial NH$_4^{+}$ uptake</td>
<td>g N m$^{-3}$</td>
<td>0.35</td>
</tr>
<tr>
<td>$K_{\text{NO}_2^{-}}$</td>
<td>M-M constant for reduction of NO$_2^{-}$ by denitrifiers</td>
<td>g N m$^{-3}$</td>
<td>1.4</td>
</tr>
<tr>
<td>$K_{\text{NO}_2^{-}}$</td>
<td>M-M constant for reduction of NO$_2^{-}$ by nitrifiers</td>
<td>g N m$^{-3}$</td>
<td>1.4</td>
</tr>
<tr>
<td>$K_{\text{NO}_3^{-}}$</td>
<td>M-M constant for oxidation of NO$_3^{-}$ by nitrifiers</td>
<td>g N m$^{-3}$</td>
<td>1.4</td>
</tr>
<tr>
<td>$K_{\text{NO}_3^{-}}$</td>
<td>M-M constant for reduction of NO$_3^{-}$ by denitrifiers</td>
<td>g N m$^{-3}$</td>
<td>0.028</td>
</tr>
<tr>
<td>$K_{\text{N}_2\text{O}_4}$</td>
<td>M-M constant for reduction of N$_2$O by denitrifiers</td>
<td>g N m$^{-3}$</td>
<td>0.064</td>
</tr>
<tr>
<td>$K_{\text{O}_2}$</td>
<td>M-M constant for reduction of O$_2$ by heterotrophs</td>
<td>g O$_2$ m$^{-3}$</td>
<td>0.064</td>
</tr>
<tr>
<td>$K_{\text{O}_2}$</td>
<td>M-M constant for reduction of O$_2$ by NH$_3$ oxidizers</td>
<td>g O$_2$ m$^{-3}$</td>
<td>0.064</td>
</tr>
</tbody>
</table>
\( K_{O_{2g}} \)  
M-M constant for reduction of O\(_2\) by NO\(_2\)^-  
g O\(_2\) m\(^{-3}\)  
[H17b]  
0.064  
Focht and Verstraete (1977) (McGill et al., 1981)

\( K_{Xh} \)  
M-M constant for oxidation of DOC by heterotrophs  
g C m\(^{-3}\)  
[H2]  
12

\( M_{i,h,a} \)  
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]

\( M_{i,m,i,C} \)  
C biomass of microbial population \( M_{i,m,i} \)  
g C m\(^{-2}\)  
[H1]

\( M_{i,m,i,N} \)  
N biomass of microbial population \( M_{i,m,i} \)  
g N m\(^{-2}\)  
[H1]

\( M_{i,a,a} \)  
active biomass of NO\(_2\)^- oxidizers  
g C m\(^{-2}\)  
[H15,H17]

\( [NH_3] \)  
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]

\( [O_{2m,h}] \)  
O\(_2\) concentration at heterotrophic surfaces  
g O\(_2\) m\(^{-3}\)  
[H7]

\( [O_{2m,n}] \)  
O\(_2\) concentration at NH\(_3\) oxidizer surfaces  
g O\(_2\) m\(^{-3}\)  
[H13]

\( [O_{2m,i,C}] \)  
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]

\( R_{NO_2/d} \)  
NO\(_2\)^- reduction by denitrifiers  
g N m\(^{-3}\) h\(^{-1}\)  
[H8,H9,H10]

\( R'_{NO_2/n} \)  
rate of NO\(_2\)^- reduction by NH\(_3\) oxidizers under non-limiting [NO\(_2\)^-] and [CO\(_2\)S]  
g N m\(^{-3}\) h\(^{-1}\)  
[H19,H20]

\( R_{NO_2/a} \)  
rate of NO\(_2\)^- reduction by NH\(_3\) oxidizers under ambient [NO\(_2\)^-] and [CO\(_2\)S]  
g N m\(^{-3}\) h\(^{-1}\)  
[H20,H21]

\( R'_{NO_3/d} \)  
NO\(_3\)^- reduction by denitrifiers under non-limiting [NO\(_3\)^-]  
g N m\(^{-3}\) h\(^{-1}\)  
[H6,H7,H8,H9]

\( R_{NO_3/d} \)  
NO\(_3\)^- reduction by denitrifiers under ambient [NO\(_3\)^-]  
g N m\(^{-3}\) h\(^{-1}\)  
[H7,H8,H9,H10]

\( R_{N_2O/d} \)  
N\(_2O\) reduction by denitrifiers  
g N m\(^{-3}\) h\(^{-1}\)  
[H9,H10]

\( R'_{O_2/d} \)  
rate of O\(_2\)S reduction by denitrifiers under non-limiting [O\(_2\)S]  
g O\(_2\) m\(^{-3}\) h\(^{-1}\)  
[H6]
Rate of O₂ reduction by denitrifiers under ambient [O₂₈] g O₂ m⁻² h⁻¹ [H6]

Rate of O₂ reduction by heterotrophs under non-limiting [O₂₈] g O₂ m⁻² h⁻¹ [H3,H4,H5]

Rate of O₂ reduction by heterotrophs under ambient [O₂₈] g O₂ m⁻² h⁻¹ [H4,H5]

Rate of O₂ reduction by NH₃ oxidizers under non-limiting [O₂₈] g O₂ m⁻² h⁻¹ [H12,H13,H14,H19]

Rate of O₂ reduction by NH₃ oxidizers under ambient [O₂₈] g O₂ m⁻² h⁻¹ [H13,H14,H19]

Rate of O₂ reduction by NO₂⁻ oxidizers under non-limiting [O₂₈] g O₂ m⁻² h⁻¹ [H16,H17,H18]

Rate of O₂ reduction by NO₂⁻ oxidizers under ambient [O₂₈] g O₂ m⁻² h⁻¹ [H17,H18]

Respiratory quotient for reduction of O₂ coupled to oxidation of C g O₂ g C⁻¹ [H3,H12,H16] 2.67 Brock and Madigan (1991)

Respiratory quotient for reduction of O₂ coupled to oxidation of NH₃ g O₂ g N⁻¹ [H12] 3.43 Brock and Madigan (1991)

Respiratory quotient for reduction of O₂ coupled to oxidation of NO₂⁻ g O₂ g N⁻¹ [H16] 1.14 Brock and Madigan (1991)

Radius of microbial sphere m [H4,H13,H17] from \( \psi_s \) according to Kemper (1966)

Radius of \( r_m \) + water film at current soil water potential m [H4,H13,H17]

Soil volume occupied by substrate-microbe complex [H6,H19]

Rate of C oxidation by NH₃ oxidizers under non-limiting [O₂₈] g C m⁻² h⁻¹ [H12]

Rate of C oxidation by NO₂⁻ oxidizers under non-limiting [O₂₈] g C m⁻² h⁻¹ [H16]

Specific rate of DOC oxidation by heterotrophs at 25 °C under non-limiting [DOC] and [O₂₈] g C g C⁻¹ h⁻¹ [H2] 0.125 Shields et al. (1973)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X'_{DOC,h}$</td>
<td>rate of DOC oxidation by heterotrophs under non-limiting $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H2,H3,H5]</td>
</tr>
<tr>
<td>$X_{DOC,h}$</td>
<td>rate of DOC oxidation by heterotrophs under ambient $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H5]</td>
</tr>
<tr>
<td>$X_{DOC,d}$</td>
<td>rate of DOC oxidation by heterotrophs under ambient $[O_2]$ and $[NO_3]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H10]</td>
</tr>
<tr>
<td>$X'_{NH_3}$</td>
<td>specific rate of NH$_3$ oxidation by NH$_3$ oxidizers at 25 °C under non-limiting $[O_2]$</td>
<td>g N g C$^{-1}$ h$^{-1}$</td>
<td>[H11]</td>
</tr>
<tr>
<td>$X_{NH_3,n}$</td>
<td>rate of NH$_3$ oxidation by NH$_3$ oxidizers coupled with reduction of O$_2$ + NO$_2^-$ under ambient $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H14,H21]</td>
</tr>
<tr>
<td>$X'_{NH_3,n}$</td>
<td>rate of NH$_3$ oxidation by NH$_3$ oxidizers under non-limiting $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H11,H12,H14]</td>
</tr>
<tr>
<td>$X'_{NO_2,o}$</td>
<td>rate of NO$_2^-$ oxidation by NO$_2^-$ oxidizers under non-limiting $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H15,H16,H18]</td>
</tr>
<tr>
<td>$X_{NO_2,o}$</td>
<td>rate of NO$_2^-$ oxidation by NO$_2^-$ oxidizers coupled with reduction of O$_2$ under ambient $[O_2]$</td>
<td>g N m$^{-2}$ h$^{-1}$</td>
<td>[H18]</td>
</tr>
<tr>
<td>$X'_{NO_2}$</td>
<td>specific rate of NO$_2^-$ oxidation by NO$_2^-$ oxidizers at 25 °C under non-limiting $[O_2]$</td>
<td>g N g C$^{-1}$ h$^{-1}$</td>
<td>[H15]</td>
</tr>
</tbody>
</table>

Belser and Schmidt (1980)

2.5 Belser (1977)
References


