Soil Organic Matter Decomposition and Nitrogen Trace Gas Calculations of the DayCent Model

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1 Introduction

The CENTURY family of models specialize in carbon and nitrogen cycling by incorporating detailed mechanistic representations of plant nutrient and water uptake, soil microbial activities, and soil organic matter evolution, and have been widely-applied to grasslands, forests, and agricultural lands around world (Parton et al. 1988, Metherell et al. 1993, Parton et al. 1993, Kelly et al. 1997, Parton et al. 2007b). The processes of the original CENTURY model operate at a monthly time step with the exception decomposition that operates at a weekly time step. The Daily Century model, or DayCent (Parton et al. 1998), was derived from the CENTURY model. Like CENTURY, DayCent has a monthly loop, but it also has a daily loop within the monthly loop for calculating plant production, soil moisture, soil temperature, decomposition, and nitrogen trace gas fluxes.

This document describes two submodels in the FORTRAN/C version DayCent along with DayCent's soil layer structure that is integral to both submodels. Chapter 2 provides and overview of the soil organic matter decomposition submodel along with detailed documentation of its calculations. Chapter 3 provides and overview of the nitrogen trace gas submodel along with detailed documentation of its calculations. The appendices define parameters for each of the parameter files: <site>.100, crop.100, cult.100, fert.100, fire.100, fix.100, graz.100, harv.100, irri.100, omad.100, tree.100, trem.100, sitpar.in, and soils.in.

1.1 Soil layer structures of the CENTURY and DayCent Models

The soil structure for monthly CENTURY model includes $1 - 10$ soil layers where the minimum thickness of any soil layer is usually no less than 15 cm. Soil layer thickness are defined by the *ADEP(*)* values in the *fix.100* parameter file. The number of actual layers used is defined by the NLAYER parameter in the *<site>.100* parameter file. The soil sand, silt, and clay fractions, along with bulk density and soil pH and are defined by the SAND, SILT, CLAY, BULKD, and PH values, respectively, in the *<site>.100* file. Field capacity and wilting point values are defined for each layer using the AFIEL(*) and AWILT(*) parameters in the *<site>.100* file.

In order to simulate daily soil water fluxes, soil temperature distribution at depth, and nitrogen trace gas fluxes, the DayCent model requires a finer soil layer structure than the CENTURY model. DayCent's developers wanted to allow for this finer soil layer structure in the soil water submodel, soil temperature submodel, and trace gas submodels without impacting other code that still required the coarser soil layer structure. Therefore, DayCent allows for multiple layers within a coarser CENTURY layer. It is important that boundaries of the layers coincide as shown in **Figure SoilLayers**. DayCent's soil layer structure and properties are defined in the *soils.in* parameter file (Table 1.1). For both models, soil layer thicknesses (cm) are defined as integer values. The *sand* and *clay* weight fractions used by the decomposition model are computed as the

weighted average their corresponding values in top 3 soil layers in *soils.in*. The organic matter weight fraction (*org*) in *soils.in* is only used in the soil temperature model. The value of *silt = 1.0 – sand – clay*, except in the soil temperature model *silt = 1.0 – sand – clay – org*. The SAND, SILT, CLAY, values entered in the *<site>.100* file are ignored. Likewise, the values BULKD, PH, AFIEL(*), and AWILT(*) in the *<site>.100* file are recalculated from values in the *soils.in* file.

Inorganic soil N is also defined differently between the CENTURY and DayCent models. The monthly CENTURY model defines 1 – 10 inorganic N layers as MINERL(*,N). In DayCent, the nitrogen trace gas submodel requires that inorganic soil N be partitioned into nitrate and ammonium in order to calculate nitrification and denitrification; inorganic N exists as a number of nitrate layers (*nitrate*(*), g N m^{-2}) that have the same thicknesses as the DayCent soil layers, plus a single *ammonium* layer that is assumed to be approximately 10 – 15 cm deep. The CENTURY *MINERL(*,*)* values are still used in portions of the DayCent code. For example, the decomposition submodel uses *MINERL(1,N)* as the labile N pool that is the source/sink for N produced from mineralization and N consumed by immobilization. *MINERL(1,N)* is equal to *ammonium* plus *nitrate(*)* from any DayCent layer that is mapped to the top CENTURY layer.

layer #	thickness (cm)	upper depth (cm)	lower depth (cm)	bulk density (g cm^{-3})	field capacity (volu-metric)	wilting point (volu-metric)	evap. coef-ficient	frac. of roots	sand frac-tion	clay frac-tion.	organic matter frac-tion	deltamim (volu-metric)	ksat (cm sec^{-1})	pH
1	2	0	2	0.83	0.1212	0.0345	0.8	0.01	0.9	0.02	0.02	0.008	0.042	4.5
2	3	2	5	0.83	0.1212	0.0345	0.2	0.04	0.9	0.02	0.02	0.008	0.042	4.5
3	5	5	10	0.83	0.1212	0.0345	0	0.25	0.9	0.01	0.02	0.008	0.042	4.5
4	10	10	20	0.83	0.1212	0.0345	0	0.3	0.9	0.01	0.02	0.008	0.042	4.5
5	10	20	30	1.01	0.1212	0.0345	0	0.1	0.9	0.02	0.02	0.008	0.042	4.5
6	15	30	45	1.01	0.125	0.0345	0	0.05	0.9	0.02	0.02	0.008	0.042	4.5
7	15	45	60	1.01	0.065	0.0345	0	0.04	0.9	0.03	0.01	0.008	0.042	4.5
8	15	60	75	1.01	0.065	0.0345	0	0.03	0.96	0.03	0.01	0.008	0.042	4.5
9	15	75	90	1.01	0.065	0.0345	0	0.02	0.96	0.03	0.01	0.008	0.042	4.5
10	15	90	105	1.23	0.065	0.0345	0	0.01	0.96	0.03	0.01	0.008	0.042	4.5
11	15	105	120	1.23	0.065	0.0345	0	0	0.96	0.03	0.01	0.008	0.042	4.5
12	30	120	150	1.23	0.065	0.0345	0	0	0.96	0.03	0.01	0.008	0.042	4.5
13	30	150	180	1.23	0.065	0.0345	0	0	0.96	0.03	0.01	0.008	0.042	4.5
14	30	180	210	1.54	0.065	0.0345	0	0	0.89	0.1	0.01	0.008	0.042	4.5

Table 1.1. An example *soils.in* parameter file for defining DayCent soil layers. (Note: the actual text file does not have a row with column names). The minimum volumetric soil water content of a layer (*swclimit*) is calculated from two columns, *swclimit = wilting point – deltamin*. The value *ksat* is the saturated hydraulic conductivity (cm sec^{-1}). The *sand* and *clay* weight fractions used by the decomposition model are computed as the weighted average their corresponding values in top 3 soil layers of this file. The organic matter weight fraction (*org*) in *soils.in* is only used in the soil temperature model. The value of *silt = 1.0 – sand – clay*, except in the soil temperature model *silt = 1.0 – sand – clay – org*. The SAND, SILT, CLAY, values in the *<site>.100* file are ignored. Likewise, the values BULKD, PH, AFIEL(*), and AWILT(*) in the *<site>.100* file are recalculated from values in the *soils.in* file. The bands of colors are to illustrate that multiple DayCent soil layers may comprise a single CENTURY soil layer.
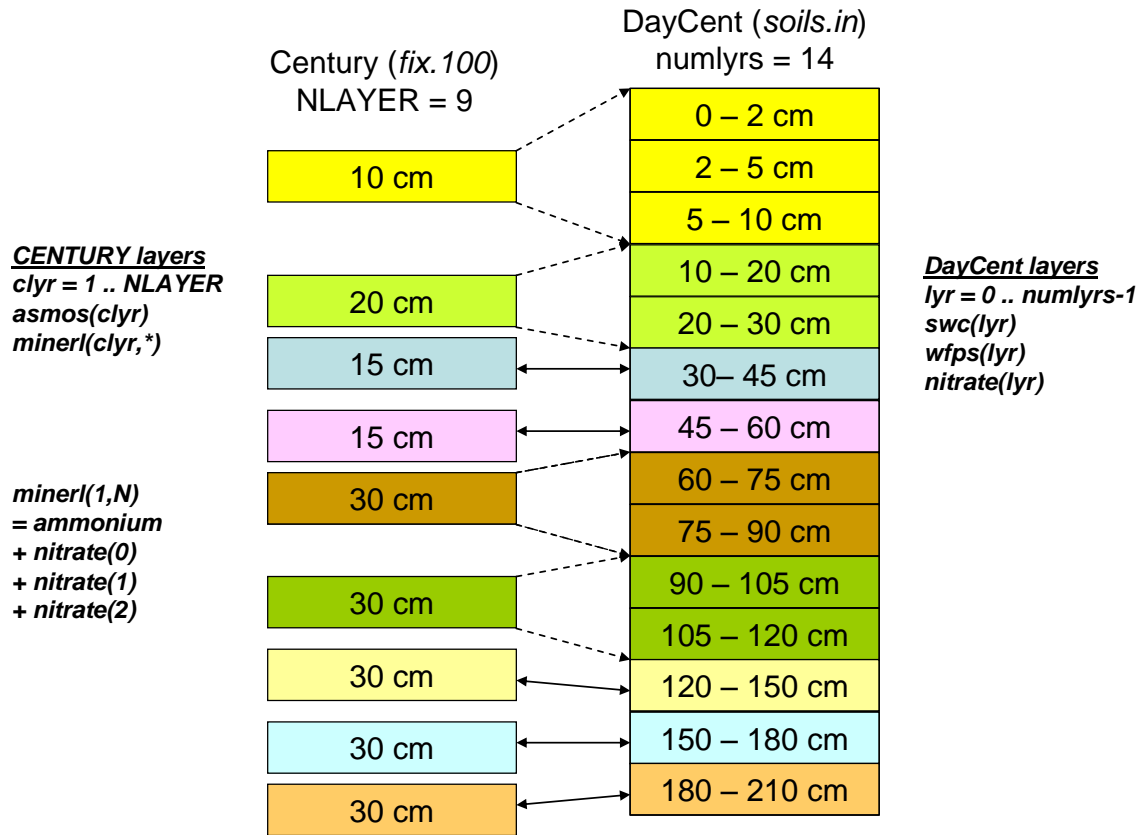
Figure SoilLayers. The relationship between "CENTURY" soil layers and finer "DayCent" soil layers. The CENTURY soil layer thicknesses are defined by *ADEP(*)* in the *fix.100* parameter file, and the number of layers to simulate is defined as *NLAYER* in the <site>.100 parameter file. The DayCent soil layers are defined in the *soils.in* parameter file (Table 1.1). There can be multiple DayCent soil layers within a CENTURY soil layer, but layer boundaries must coincide as illustrated. The soil thicknesses shown above are for example; actual values are defined by the user.

2 Decomposition

2.1 Intrinsic Rates of Decomposition

The decomposition submodel of DayCent operates at a daily timestep, while the intrinsic rates of decomposition are specified in the *fix.100* parameter file as annual rates (yr^{-1}) (Table 2.1). To calculate the daily rate of decomposition, the annual rates are multiplied by the decomposition time step (*dtm*, fraction of a year). For example, the annual rate (k_{An}, yr^{-1}) is converted to a daily rate (k_{Day}, day^{-1}) as

$$k_{Day} = k_{An} \times dtm \tag{2.1}$$

$$dtm = \frac{1}{12 \times daysInMonth(imo)} \tag{2.2}$$

where *daysInMonth(imo)* is the number of days in the current month (*imo* = 1,12). While this is not the best way to compute a daily rate from an annual rate, it is similar to the monthly timestep version of the CENTURY model that also multiplies the annual rate by *dtm*, where *dtm* = 1/12.

To run the decomposition model more than once a day, a different function is used to convert the decomposition rates. In general, k_1 is the discrete-time decomposition rate for a timestep of Δt_1 minutes, and k_2 is the discrete-time decomposition rate for a timestep of Δt_2 minutes. If *k1*, Δt_1, and Δt_2 are known, then k_1 is converted to a continuous-time rate (k_{cont}), and k_2 is calculated following Olson (1963):

$$k_{cont} = -\log(1.0 - k_1) \qquad\qquad k_1 \leq 1.0$$

$$k_2 = 1.0 - \exp\left(-k_{cont} \times \frac{\Delta t_2}{\Delta t_1}\right) \tag{2.3}$$

$$k_2 = k_1 \times \frac{\Delta t_2}{\Delta t_1} \qquad\qquad k_1 > 1.0$$

where log is the natural logarithm function (the inverse of exp). For example, to calculate the discrete-time rate for a 30 minute timestep from of a daily timestep, set Δt_2 = 30 minutes, Δt_1 = 24 x 60 minutes (a day), and $k_1 = k_{An}$ x *dtm* (Eqs. 2.1 and 2.2).

Variable	Description	k (yr^{-1})	*Turnover time*
strucc(1)	surface structural litter	2	0.5 yr
strucc(2)	soil structural litter	4.9	74 days
metabc(1)	surface metabolic litter	8	46 days
metabc(2)	soil metabolic litter	18.5	20 days
som1c(1)	active surface organic matter	6	61 days
som1c(2)	active soil organic matter	11	33 days
som2c(1)	slow surface organic matter	0.08	12.5 yr
som2c(2)	slow soil organic matter	0.4	2.5 yr
som3c	passive soil organic matter	0.0033	303 yr

Table 2.1. Maximum decomposition rates, k (yr^{-1}), and turnover times for litter and organic matter pools.

2.2 Variable Definitions

2.2.1 Components of organic matter pools, mineral pools, and plant pools

The following abbreviations are indices for arrays used by the DayCent model.

SRFC – index for the surface component of a pool (above ground) (*SRFC* = 1)
SOIL – index for soil component of a pool (below ground) (*SOIL* = 2)
lyr – index for the SRFC or SOIL component of an organic pool (*lyr* = 1, 2) or the index for any of the *n* mineral soil layers (*lyr* = 1, .., *n*)

N – index for a nitrogen pool (N = 1)
P – index for a phosphorus pool (P = 2)
S – index for a sulfur pool (S = 3)
E – abbreviation for the element N, P, or S.
iel – index for the N, P, and S components of a pool (*iel* = 1, 2, 3)

In addition to carbon, DayCent can be specified to simulate 1, 2, or 3 other elemental pools. The number of additional elements to simulate is specified by the NELEM parameter in the <site>.100 file. If NELEM = 1, nitrogen is simulated. If NELEM = 2, then nitrogen and phosphorus are simulated. If NELEM = 3, then nitrogen, phosphorus, and sulfur are simulated. Therefore, carbon and nitrogen are always simulated, and phosphorous and sulfur are optional.

UNLABL – index for the unlabeled component of an organic matter pool
LABELD – index for the labeled component of an organic matter pool

SLOPE – index for the SLOPE term for a linear equation (*SLOPE* = 1)
INTCPT – index for the INTERCEPT term for a linear equation (*INTCPT* = 2)

CPARTS – number of crop/grass components (*CPARTS* = 3)
ABOVE – index for the above ground component of a crop/grass (*ABOVE* = 1)
BELOWJ – index for the juvenile fine root component of a crop/grass (*BELOWJ* = 2)
BELOWM – index for the mature fine root component of a crop/grass (*BELOWM* = 3)

FPARTS – number of tree/shrub components (*FPARTS* = 6)
LEAF – index for the leaf component of a tree/shrub (*LEAF* = 1)
FBRCH – index for the leaf component of a tree/shrub (*FBRCH* = 3)
LWOOD – index for the large wood component of a tree/shrub (*LWOOD* = 4)
FROOTJ – index for the juvenile fine component of a tree/shrub (*FROOTJ* = 2)
FROOTM – index for the mature fine root component of a tree/shrub (*FROOTM* = 6)
CROOT – index for the coarse root component of a tree/shrub (*CROOT* = 5)

Note: *FBRCH*, *LWOOD*, and *CROOT* are woody components, the other tree/shrub components are non-woody.

2.2.2 Litter C, N, P, and S pools

metabc(SRFC) – unlabeled and labeled C of surface metabolic litter (g C m^{-2})
        = *metcis(SRFC,UNLABL) + metcis(SRFC,LABELD)*
metabe(SRFC,iel) – N, P, or S component of surface metabolic litter pool (g E m^{-2})

metabc(SOIL) – unlabeled and labeled C of soil metabolic litter (g C m^{-2})
        = *metcis(SOIL,UNLABL) + metcis(SOIL,LABELD)*
metabe(SOIL,iel) – N, P, or S component of soil metabolic litter (g E m^{-2})

strucc(SRFC) – unlabeled and labeled C of surface structural litter (g C m^{-2})
        = *strucis(SRFC,UNLABL) + strucis(SRFC,LABELD)*
struce(SRFC,iel) – N, P, or S component of surface structural litter (g E m^{-2})

strucc(SOIL) – unlabeled and labeled C of soil structural litter (g C m^{-2})
        = *strucis(SOIL,UNLABL) + strucis(SOIL,LABELD)*
struce(SOIL,iel) – N, P, or S component of soil structural litter (g E m^{-2})

strlig(SRFC) – lignin content of surface structural litter (g lignin C / g C)
strlig(SOIL) – lignin content of soil structural litter (g lignin C / g C)

2.2.3 Soil organic matter C, N, P, and S pools

som1c(SRFC) – unlabeled and labeled C in the active surface pool (surface microbes with fast turnover) (g C m^{-2})
        = *som1ci(SRFC,UNLABL) + som1ci(SRFC,LABELD)*
som1e(SRFC,iel) – N, P, or S component of the active surface pool (g E m^{-2})

som1c(SOIL) – unlabeled and labeled C in the active soil pool (soil microbes with fast turnover) (g C m^{-2})
= *som1ci(SOIL,UNLABL) + som1ci(SOIL,LABELD)*
som1e(SOIL,iel) – N, P, or S component of the active soil pool (g E m^{-2})

som2c(SRFC) – unlabeled and labeled C of the slow surface pool (with intermediate turnover) (g C m^{-2})
= *som2ci(SRFC,UNLABL) + som2ci(SRFC,LABELD)*
som2e(SRFC,iel) – N, P, or S component of the slow surface pool (g E m^{-2})

som2c(SOIL) – unlabeled and labeled C of the slow soil pool (with intermediate turnover) (g C m^{-2})
= *som2ci(SOIL,UNLABL) + som2ci(SOIL,LABELD)*
som2e(SOIL,iel) – N, P, or S component of the slow soil pool (g E m^{-2})

som3c – unlabeled and labeled C of the passive soil pool (with the slowest turnover) (g C m^{-2})
= *som3ci(UNLABL) + som3ci(LABELD)*
som3e(iel) – N, P, or S component of the passive soil pool (g E m^{-2})

2.2.4 Dead wood C, N, P, and S pools

wood1c – unlabeled and labeled C of dead fine branches (g C m^{-2})
= *wd1cis(UNLABL) + wd1cis(LABELD)*
wood1e(iel) – N, P, or S component of dead fine branches (g E m^{-2})

wood2c – unlabeled and labeled C of dead large wood (g C m^{-2})
= *wd2cis(UNLABL) + wd2cis(LABELD)*
wood2e(iel) – N, P, or S component of dead large wood (g E m^{-2})

wood3c – unlabeled and labeled C of dead coarse roots (g C m^{-2})
= *wd3cis(UNLABL) + wd3cis(LABELD)*
wood3e(iel) – N, P, or S component of dead coarse roots (g E m^{-2})

wdlig(*) – lignin content of the 6 tree/shrub parts (g lignin C / g C)

2.2.5 Plant C pools that are cycled into above and below ground litter pools

Crops, grasses, and other herbaceous vegetation

aglivc – carbon in above ground live shoots (g C m^{-2})
bglivcj – carbon in below ground live juvenile fine roots (g C m^{-2})

bglivcm – carbon in below ground live mature fine roots (g C m^{-2})
stdedc – carbon in standing dead plants (g C m^{-2})

Trees, shrubs, and other woody vegetation

rleavc – carbon in live leaves (g C m^{-2})
frootcj – carbon in live juvenile fine roots (g C m^{-2})
frootcm – carbon in live mature fine roots (g C m^{-2})
fbrchc – carbon in live fine branches (g C m^{-2})
lwoodc – carbon in live large wood (g C m^{-2})
crootc – carbon in live coarse roots (g C m^{-2})

Note: *fbrchc, lwoodc,* and *crootc* are woody components. The others are non-woody.

2.2.6 Constants

biocnv – factor to convert carbon to biomass for all organic material but wood
        (2.5 g biomass / g C)

woodcnv – factor to convert wood carbon to wood biomass
        (2.0 g biomass / g C)

2.3 Overview of the Soil Organic Matter Submodel

The soil organic matter submodel of the DayCent model is based on multiple compartments for soil organic matter (Parton et al. 1987). The model includes three soil organic matter pools (active, slow and passive) with different potential decomposition rates. Plant material is transferred into these soil organic matter pools from above and belowground litter pools and three dead wood pools (**Figures DecompC and DecompN**). Both the active and the slow organic matter pools have a surface and soil component while the passive pool has only a soil component.

Above and belowground non-woody plant residues and organic animal excreta are partitioned into structural (STRUCC(*)) and metabolic (METABC(*)) pools as a function of the lignin to N ratio in the residue. Structural material is assumed to contain cellulose and all of the lignin whereas metabolic material is readily decomposable. With increases in the ratio, more of the residue is partitioned to the structural pools which have much slower decay rates than the metabolic pools (**Figures Residue, Partition**). Metabolic pools are decomposed primarily by bacteria while structural pools are decomposed primarily by fungi. Dead wood pools (WOOD1C, WOOD2C, and WOOD3C) decompose directly into the active pools (SOM1C(*)), and the slow pools (SOM2C(*)). The decomposition rate of the structural material (STRUCC(*)) is a function of the fraction of the structural material that is lignin, and the decomposition of

dead wood (WOOD1C, WOOD2C, and WOOD3C) is a function of the fraction of wood that is lignin.

The abiotic process of photodecomposition, where incoming solar radiation accelerates the decomposition of dead plant material, may be and important process in arid grasslands (Parton et al. 2007a, Adair et al. 2008). The loss of C from the standing dead pool (STDEDC) or from the surface structural (STRUCC(1)) is proportional to the amount of solar radiation each absorbs. Photodegradation of STDEDC results in a CO_2 loss without nutrient loss. Photodegradation of STRUCC(1) results in a CO_2 loss as well as a flow of C to surface metabolic METABC(1), with some nutrient flow from STRUCE(*) to METABE(*).

Aside from photodecomposition, the decomposition of both plant residues and soil organic matter are assumed to be microbially mediated with an associated loss of CO_2 as a result of microbial respiration. Decomposition products flow into a surface active pool (SOM1C(1)), the surface slow pool (SOM2C(1), or one of three soil organic matter pools (SOM1C(2), SOM2C(2), and SOM3C), each characterized by different maximum decomposition rates.

The active surface pool (SOM1C(1) and active soil pool (SOM1C(2)) represent soil microbes and microbial products (total active pool is ~2 to 3 times the live microbial biomass level) and have a turnover time of months to a few years depending on the environment. The soil texture influences the turnover rate of the active SOIL organic matter (higher rates for sandy soils) and the efficiency of stabilizing active SOIL organic matter into slow SOIL organic matter (higher stabilization rates for clay soils). The surface microbial pool (SOM1C(1)) turnover rate is independent of soil texture, and it transfers material directly into the surface slow soil organic matter pool (SOM2C(1)).

The slow surface pool (SOM2C(1)) and slow soil pool (SOM2C(2) include resistant plant material derived from the structural pool. The soil slow pool (SOM2C(2)) also includes soil-stabilized microbial products derived from the active soil pool. These pools have a turnover time of a couple years to a decade or more. There is a transfer of SOM2C(1) to SOM2C(2) due to physical mixing. The transfer of SOM2C(2) to SOM1C(2) is probably not very important (5%), and most of this flow results in a CO_2 loss.

The passive soil pool (SOM3C) is very resistant to decomposition and includes physically and chemically stabilized soil organic matter and has a turnover time of 300 to 1000 years. The proportions of the decomposition products which enter the passive pool from the slow and active pools increase with increasing soil clay content. The stabilization of the active soil pool is the primary source for the passive pool. Some passive SOM is also created by the decomposition of slow organic matter. There is no transfer of surface litter or SOM1C(1) to SOM3C. Flows to SOM3C occur in only in the soil.

The potential decomposition rates of surface and soil pools (Table 2.1) are reduced by multiplicative functions (DEFAC) of soil moisture and soil temperature. Average daily soil temperature near the soil surface (STEMP) is the input for the temperature function. The soil temperature effect on decomposition is computed as variable Q_{10} function, with low Q_{10} values at high temperatures and high Q_{10} values at low temperatures (Del Grosso et al. 2005) (**Figure TFUNC**). The IDEF parameter (*fix.100*) determines the if the moisture function uses relative water content **(Figure WFUNCa)**, the ratio of stored soil water (0-30 cm depth, AVH2O(3)) plus current day's precipitation to potential evapotranspiration (PET) **(Figure WFUNCa)**, or water-filled pore space and soil texture **(Figure WFUNCb)**.

The potential decomposition rate of surface and soil pools is also reduced by the effect soil pH on the dominant type of decomposer (**Figure PH**). Fungi are the dominant composer for SOM3C, and bacteria are the primary composer for METABC. For all other pools, SOM1C(*), SOM2C(*), STRUCC(*), WOOD1C, WOOD2C, and WOOD3C, a combination of fungi and bacteria is used. The potential decomposition of soil pools can be further reduced by the effect of anaerobic conditions (high soil water content) (ANERB) (**Figure ANERB**), or increased as an effect of cultivation (CLTEFF(*), *cult.100*). The soil drainage factor (DRAIN, *<site>.100*) allows a soil to have differing degrees of wetness (e.g., DRAIN=1 for well drained sandy soils and DRAIN=0 for a poorly drained clay soil).

A fraction of the products from the decomposition of the active pool is lost as leached organic C (STREAM(5)). Leaching of organic matter is a function of the decay rate for active soil organic matter, and the clay content of the soil (less loss for clay soils) and only occurs if there is drainage of water below the 20 cm soil depth. Leaching loss increases with increasing water flow up to a critical level - OMLECH(3), *fix.100*).

The model has N, P, and S pools analogous to the C pools (**Figure DecompN**). Each soil organic matter pool has an allowable range of C to element (C/E) ratios based on the conceptual model of McGill and Cole (1981). Reflecting the concept that N is stabilized in direct association with C, C/N ratios are constrained within narrow ranges, while the ester bonds of P and S allow C/P and C/S ratios to vary widely. The ratios in the structural pool are fixed at high values, while the ratio in the metabolic pool is allowed to float in concert with the nutrient content of the plant residues. The N, P, and S flows between soil organic matter pools are related to the C flows. The quantity of each element flowing out of a particular pool equals the product of the C flow and the element to C ratio of the pool. The C/E ratios for material entering each destination soil organic matter pool are linear functions of the labile inorganic mineral pools in the surface soil layer (MINERL(1,*)) (**Figure DRAT**). Low nutrient levels in the labile pools result in high C/E ratios in the various soil organic matter pools. Mineralization or immobilization of N, P, and S occurs as is necessary to maintain the C/E ratios required for the destination pool. Thus, mineralization of N, P, and S occurs as C is lost in the form of CO_2 and as C flows from pools with low C/E ratios, such as the active pool, to those with higher C/E ratios, such as the slow pool. Immobilization occurs when C flows from pools with high C/E ratios, such as the structural pool, to those with lower C/E ratios,

such as the active pool; the maximum amount of immobilization occurs when aminrl(iel) is greater than VARAT(3) and the C/E ratio of the destination pool is at a minimum (**Figure DRAT**). The decomposition will not occur if the quantity of any element is insufficient to meet the immobilization demand. The initial content of N in plant litter is very important. Low litter N leads to immobilization while high litter N leads to mineralization (Parton et al. 2007a).
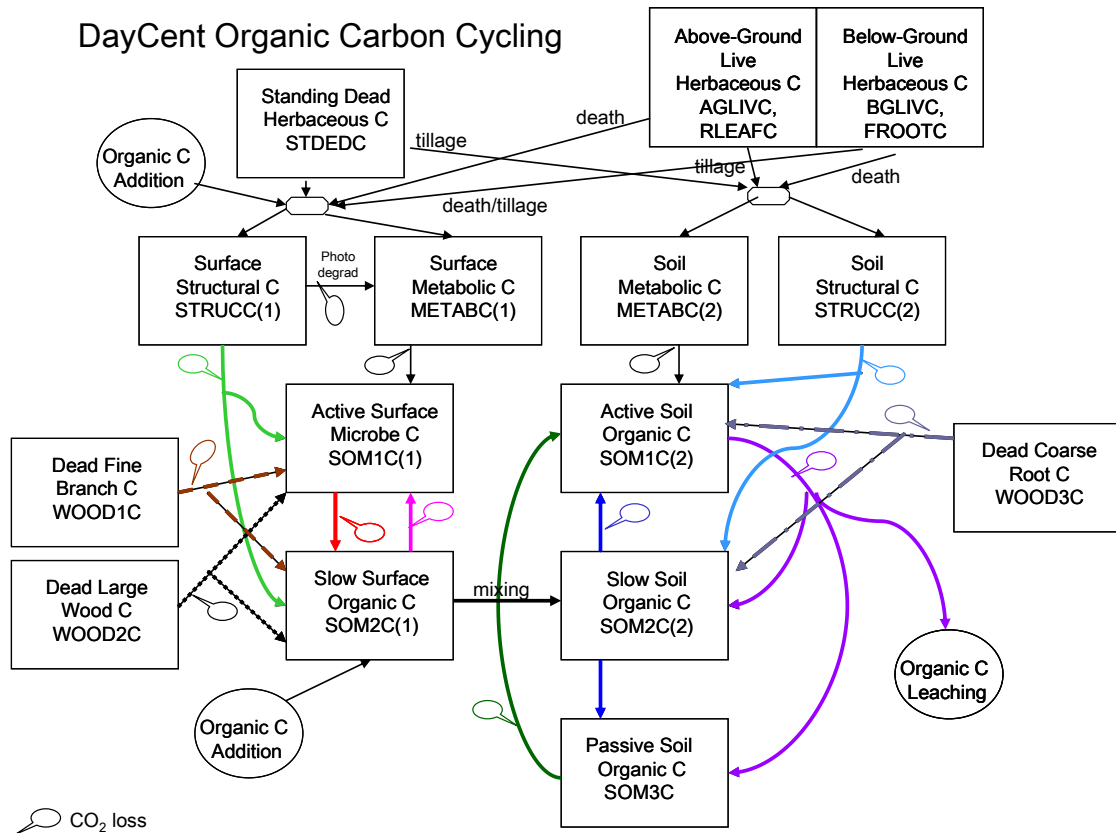
Figure DecompC. An overview of the decomposition carbon flows between the organic matter pools and the associated respiration and organic C leaching losses. Non-woody plant residue and other organic C additions are partitioned into structural (*STRUCC(*)*) and metabolic litter (*METABC(*)*) (**Figure Residue**). Partially decomposed organic C (such as compost) can be added directly to SOM2C(1). When woody plants die, their dead wood is added directly to *WOOD1C*, *WOOD2C*, and *WOOD3C*. Losses of C from plant harvest, grazing, and fire are not shown.
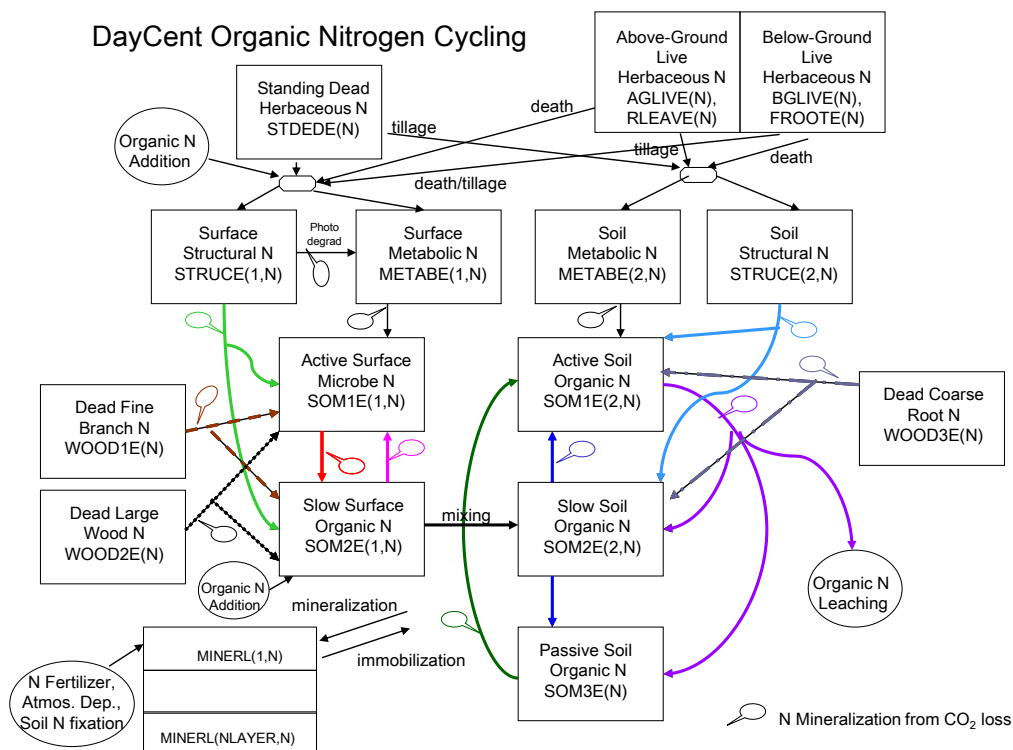
Figure DecompN. An overview of the decomposition nitrogen flows between the organic matter pools and the associated mineralization and organic N leaching losses. Non-woody plant residue and other organic N additions are partitioned into structural (*STRUCE(*,N))* and metabolic litter (*METABE(*)).* Partially decomposed organic N (such as compost) can be added directly to SOM2E(1,N). When woody plants die, their dead wood is added directly to *WOOD1E(N)*, *WOOD2E(N)*, and *WOOD3E(N)*. Any N mineralization that occurs is added to MINERL(1,N), while any N immobilization that occurs is removed from MINERL(1,N). Inorganic N additions such as N fertilizer, atmospheric N deposition, and non-symbiotic soil N fixation are added to MINERL(1,N). Losses of N from plant uptake, plant harvest, grazing, fire, inorganic N leaching, N volatilization, and N trace gas fluxes are not shown. Symbiotic N fixation is also not shown.

2.4 Partitioning of non-woody plant residue to litter pools (partit.f)

Residue from dead non-woody plant material must be partitioned into above and below ground litter pools before it can be incorporated into soil organic matter. This is accomplished by the subroutine partit that partitions the plant residue into structural (*strucc*) and metabolic (*metabc*) litter pools (**Figure Residue**).

Partitioning non-woody plant residue into litter pools
Includes residue from fine roots, leaves, grasses, and organic matter additions
(subroutine partit)

cdonor

edonor(iel)

frlign = fraction of lignin in cpart

frmet = f(lignin/N)

epart(iel) =
cpart * recres(iel)

minerl(1,iel)

dirabs(iel)

cpart

cadds =
cpart - caddm

caddm =
frmet * cpart

strucc(lyr)

struce(lyr,iel)

metabc(lyr)

metabe(lyr,iel)

eadds =
cadds / rcestr(iel)

eaddm = epart(iel) +
dirabs(iel) - eadds

rcestr(iel) is the C/E ratio of structural material (fix.100 parameter)

Figure Residue. The partitioning of non-woody plant residue into structural and metabolic litter pools. The carbon that flows (*cpart*) from the C component of plant residue (*cdonor*) is partitioned into the structural C (*strucc(lyr)*) and metabolic C (*metabc(lyr)*) litter pools. The N, P, and S that flows (*epart(iel)*) with possible direct absorption (*dirabs(iel)*) from the N, P, or S component of plant residue (*edonor(iel)*) is partitioned into structural E (*struce(lyr,iel)*) and metabolic E (*metabe(lyr,iel)*) litter pools. The value of *epart(iel)* is determined from the amount of *cpart* and the E to C ratio of the residue (*recres(iel)*). The fraction of *cpart* that flows into metabolic litter (*frmet*) is dependent on the lignin:N ratio of the residue (**Figure Partition**). The value *caddm* is the

18

portion of *cpart* that flows into *metabc(lyr)* while *cadds* is the portion that flows into *strucc(lyr)*. The value *eaddm* is the portion of *epart(iel)* that flows into *metabe(iel)* while *eadds* is the portion that flows into *struce(iel)*. The value *rcestr(iel)* is the C/E ratio of structural material (*fix.100*).

**Fraction of plant residue flowing into *metabc (frmet)*
based on the ratio of lignin to N of incoming residue *(rlnres)*
spl(INTCPT) = 0.85
spl(SLOPE) = -0.013**
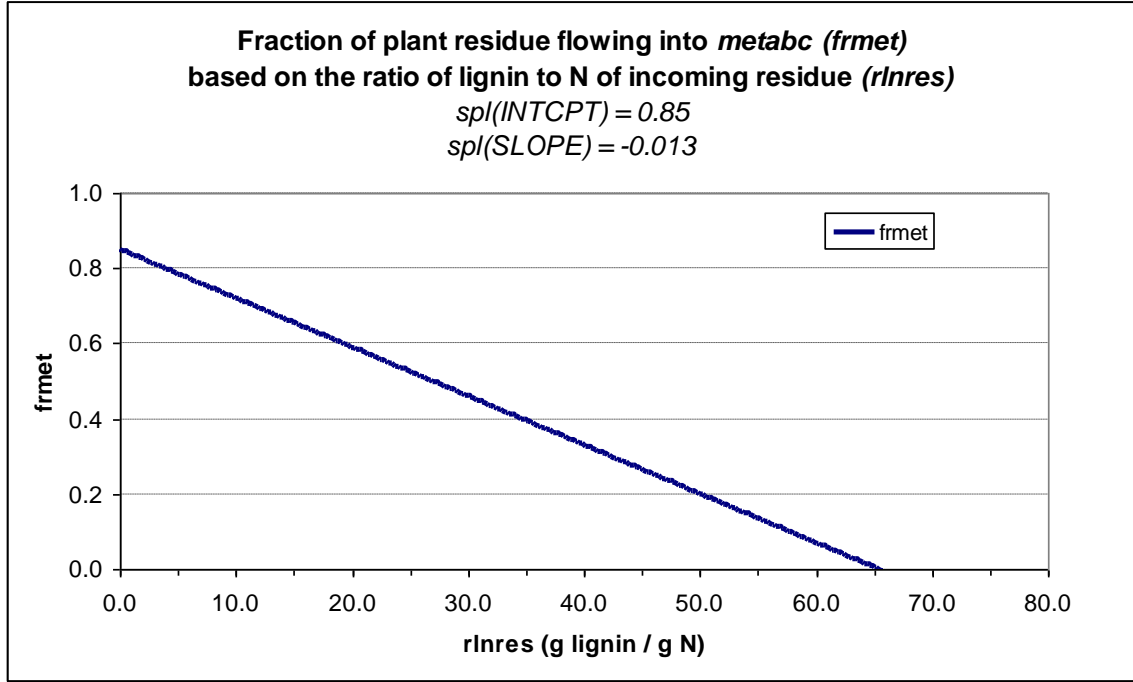
Figure Partition. The fraction of organic residue that is partitioned to the metabolic litter pool (*frmet*) decreases linearly as the ratio of lignin to N in the incoming residue (*rlnres,* g lignin biomass / g N) increases. The remaining fraction of the residue (1 – *frmet*) is partitioned to the structural litter pool. For this example, *spl(INTCPT)* = 0.85 and *spl(SLOPE)* = -0.013. The values *spl(INTCPT)* and *spl(SLOPE)* are *fix.100* parameters. Note: a positive value of SPL(2) in *fix.100* is negated in the code to create a negative slope; do not assign SPL(2) a negative number.

The value c*part* is the amount of carbon in the residue (g C m^{-2}) that is to be transferred to *strucc(lyr)* and *metabc(lyr)*. *Cpart* is transferred to *strucc(SRFC)* and *metabc(SRFC)* if the residue is from an above ground source such as *aglivc, stdedc,* or organic matter additions; it is transferred to *strucc(SOIL)* and *metabc(SOIL)* if it is from a below ground source such as *bglivcj, bglivcm, frootcj,* or *frootcm.* The initial value of the elemental component of this residue (*epart(iel)*, g E m^{-2}) is computed as

$$epart(iel) = cpart \times recres(iel) \tag{2.4}$$

where *recres(iel)* is the E/C ratio of the residue.

While partitioning the plant residue, the model assumes that fractions of soil mineral N are immobilized, and in effect modify the lignin to N ratio. This direct absorption of mineral element by residue (*dirabs*, g E m^{-2}) is calculated as

$$dirabs(iel) = damr(lyr, iel) \times minerl(1, iel) \times \max\left(\frac{cpart}{pabres}, 1.0\right) \tag{2.5}$$

where *damn(lyr,iel)* is the fraction of surface or soil E absorbed by residue (*fix.100. 0.0 – 0.1*), *minerl(1,iel)* is the mineral E in the top layer of soil (g E m^{-2}), and *pabres* is amount of residue which will give maximum direct absorption of N (g C m^{-2}, *fix.100*).

If C/E ratio of the residue flow, *rcetot*, is less than the minimum C/E ratio allowed in residue after direct absorption (*damrmn(iel)*, *fix.100*), the amount *dirabs(iel)* is reduced so that the C/E of residue is equal to *damrmn(iel)*.

$$rcetot = \frac{cpart}{epart(iel) + dirabs(iel)} \tag{2.6}$$

$$dirabs(iel) = \max\left(\frac{cpart}{damrmn(iel)} - epart(iel),\ 0.0\right),\ rcetot(iel) < damrmn(iel) \tag{2.7}$$

The lignin:N ratio of residue (*rlnres*, g lignin biomass / g N) is calculated as

$$rlnres = frlign \times \frac{cpart \times biocnv}{epart(N) + dirabs(N)} \tag{2.8}$$

where *frlign* is the lignin fraction of the residue (g lignin C / g residue C), and *biocnv* is a factor to convert carbon to biomass for all organic material but wood (2.5 g biomass / g C).

The fraction of residue carbon that goes to *metabc* (*frmet*, 0.20 – 1.0) is computed as

$$frmet = \max(spl(INTCPT) - spl(SLOPE) \times rlnres, 0.20) \tag{2.9}$$

where *rlnres* is the lignin:N ratio of residue (g lignin biomass / g N, Eq. 2.8), and *spl(INCPT)* and *spl(SLOPE)* are *fix.100* parameters (**Figure Partition**). (Note: a positive value of SPL(2) in *fix.100* is negated in the equation above to create a negative slope; do not enter SPL(2) a negative number). Readjust *frmet* if the lignin fraction of residue (*frlign,* g lignin C / g residue C) is greater than the fraction which goes to structural (1.0 - *frmet*); in other words, *frmet* cannot be greater than the non-lignin fraction of residue (1 – *frlign*) is less than *frmet*:

$$frmet = \min(frmet,\ 1.0 - frlign) \tag{2.10}$$

The amount of residue carbon flowing to *metabc(lyr)* (*caddm*, g C m^{-2}) and the amount of residue carbon flowing to *strucc(lyr)* (*cadds*, g C m^{-2}) are computed as

$$caddm = cpart \times frmet \tag{2.11}$$

$$\begin{aligned} cadds &= cpart - caddm \\ &= cpart \times (1.0 - frmet) \end{aligned} \tag{2.12}$$

After partitioning the residue, the lignin content structural material (*strlig(lyr)*, g lignin C / g C) must be updated based on the new C flow into *strucc(lyr)* (*cadds*, g C m^{-2}). The fraction of lignin in *cadds* (*fligst*, g lignin C / g residue C) can be calculated based on the assumption that all of the lignin that was in plant residue ends up in *cadds*,

$$fligst \times cadds = frlign \times cpart \tag{2.13}$$

where *cpart* is the total amount of residue (g C m^{-2}), and *frlign* is the lignin fraction of the residue *(*g lignin C / g residue C). Solving for *fligst*,

$$fligst = \min\left(\frac{frlign}{\left(\dfrac{cadds}{cpart} \right)},\ 1.0 \right) \tag{2.14}$$

In subroutine adjlig, the new value of *strlig(lyr),* the lignin fraction of structural material (g lignin C / g C), is calculated from its previous value, the amount of *strucc* before the addition of *cadds*, and the lignin fraction of *cadds (fligst),* and *cadds.*,

$$strlig(lyr) = \frac{strlig(lyr) \times strucc(lyr) + fligst \times cadds}{strucc(lyr) + cadds} \tag{2.15}$$

where *strlig(lyr) x strucc(lyr)* is the previous amount of lignin C in structural material, *fligst x cadds* is the amount of lignin C that will be added to structural material, and *strucc + cadds* in the new amount of total C in structural material.

The elemental flow into *struce(lyr,iel)* (*eadds*, g E m^{-2}) and the elemental flow into *metabe(lyr,iel)* (*eaddm*, g E m^{-2}) are computed as

$$eadds = \frac{cadds}{rcestr(iel)} \tag{2.16}$$

$$eaddm = epart(iel) + dirabs(iel) - \; eadds \tag{2.17}$$

where *rcestr(iel)* is the C/E ratio of structural material (*fix.100*), and *dirabs(iel)* is the amount of direct absorption from *minerl(1,iel)* (g E m^{-2}, Eqs. 2.5 and 2.7).

2.5 Functions Used for Decomposition Calculations

2.5.1 Line function (linear interpolation)

The *line* function returns a value of *y* from the (*x, y*) coordinate that lies on the line containing points (*x1,y1*) and (*x2, y2*) .

$$y = \text{line}(x, x1, y1, x2, y2)$$

The value of *y* is calculated as

$$y = \frac{y2 - y1}{x2 - x1} \times (x - x2) + y2 \tag{2.18}$$

2.5.2 Abiotic Decomposition Factor (*agdefac* and *bgdefac*)

Soil temperature and soil moisture affect the rate of soil decomposition. The abiotic decomposition factor ($0 \leq defac \leq 1$) is a product of a temperature effect on decomposition (*tfunc*) and a moisture effect on decomposition (*wfunc*).

$$defac = tfunc \times wfunc \tag{2.19}$$

When calculated for aboveground decomposition it is called *agdefac*, for belowground decomposition it is called *bgdefac*. Minimum decomposition rates occur when the value of *defac* is near zero, while the maximum rate of decomposition occurs when the value of *defac* is 1.0.

The temperature effect on decomposition (*tfunc*) is a variable Q_{10} function and is computed as

$$tfunc = \frac{teff_2 + \dfrac{teff_3}{\pi}\arctan\left(\pi \times teff_4\left(soiltemp - teff_1\right)\right)}{normalizer}$$

$$normalizer = teff_2 + \frac{teff_3}{\pi}\arctan\left(\pi \times teff_4\left(30.0 - teff_1\right)\right) \tag{2.20}$$

$$tfunc = \max(tfunc, 0.01)$$

where *soiltemp* is the average surface soil temperature for the day, *teff₁* – *teff₄* are *fix.100* parameters, and *normalizer* is the value of the *tfunc* numerator when *soiltemp* = 30 ºC. The function has a low Q_{10} values at high temperatures and high Q_{10} values at low temperatures (Del Grosso et al. 2005). The value of *tfunc* is the same for surface and soil decomposition.
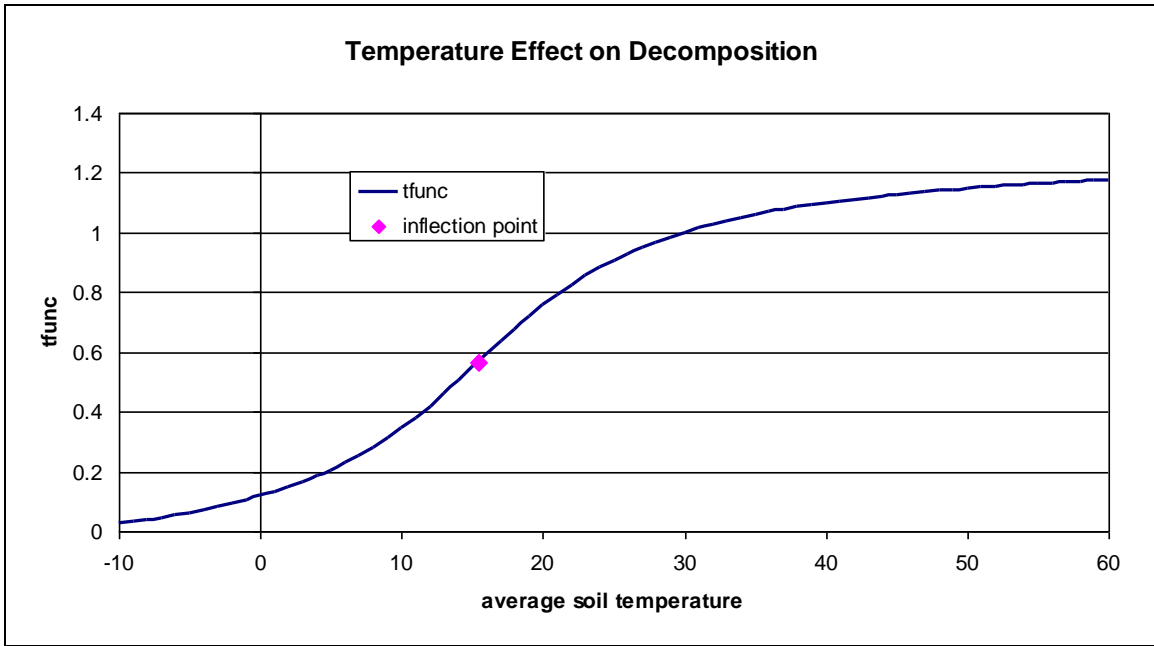
Figure TFUNC. The variable Q_{10} temperature effect on decomposition (*tfunc*) with *teff₁* = 15.4, *teff₂* = 11.75, *teff₃* = 29.7, and *teff₄* = 0.031. The value of *tfunc* strictly increases with average soil temperature, but has a low Q_{10} values at high temperatures and high Q_{10} values at low temperatures. The *teff₁* parameter determines the x-location of the inflection point. See also Del Grosso, Parton et al. (2005) that expresses this function without the *normalizer* in the denominator as in Eq. 2.20.

The moisture effect on decomposition (*wfunc*) is computed in one of three ways, depending on the value of the *fix.100* parameter IDEF (1, 2, or 3).

When IDEF = 1, the relative water content of soil controls the moisture effect. The relative water content of a soil layer, *relWaterContent$_{lyr}$*, is computed as

$$relWaterContent_{lyr} = \frac{vswc_{lyr} - swclimit_{lyr}}{fieldc_{lyr} - swclimit_{lyr}} \text{、} \tag{2.21}$$

where *vswc$_{lyr}$* is the volumetric soil water content of the layer, *fieldc$_{lyr}$* is the volumetric soil water content at field capacity, and *swclimit$_{lyr}$* is the volumetric fraction that can never be extracted from the soil layer (**Figure WFUNCa**).

$$wfunc = \frac{1.0}{1.0 + 30 \times \exp(-9.0 \times relWaterContent)} \tag{2.22}$$

For aboveground decomposition, *relWaterContent* is the relative water content of the top soil water layer. For belowground decomposition, *relWaterContent* is the weighted average relative soil water content of the second and third soil water layers.

When IDEF =2, the ratio of available water to potential evapotranspiation (*rprpet*) controls the moisture effect on decomposition (**Figure WFUNCa**). The value *rprpet* is calculated from the amount of rainfall (*rain*, cm day^{-1}), the amount of snow melt (*melt*, cm day^{-1}), the amount of available water above wilting point in the top two Century soil layers (*avh2o(3)*, cm), and the potential evapotranspiration (*PET*, cm day^{-1}). In this case, *wfunc* is the same for above and belowground decomposition; therefore, *agdefac* = *bgdefac*.

$$rprpet = \frac{rain + melt + avh2o(3)}{PET} \tag{2.23}$$

$$wfunc = \frac{1.0}{1.0 + 30 \times \exp(-8.5 \times rprpet)} \tag{2.24}$$

When IDEF = 3, soil texture and the average water filled pore space of the top three soil water layers (*wfps$_{avg}$*) controls the moisture effect on decomposition (**Figure WFUNCb**). In this case, *wfunc* is the same for above and belowground decomposition; therefore, *agdefac* = *bgdefac*.

$$
\begin{aligned}
base1 &= \frac{wfps_{avg} - b}{a - b} \\
base2 &= \frac{wfps_{avg} - c}{a - c} \\
wfunc &= base1^{d\left(\frac{b-a}{a-c}\right)} \times base2^{d}
\end{aligned}
\tag{2.25}
$$

When the soil is coarse, a = 0.55f, b = 1.70, c = -0.007, and d = 3.22. When the soil is medium or fine textured a = 0.60, b = 1.27, c = 0.0012, and d = 2.84.
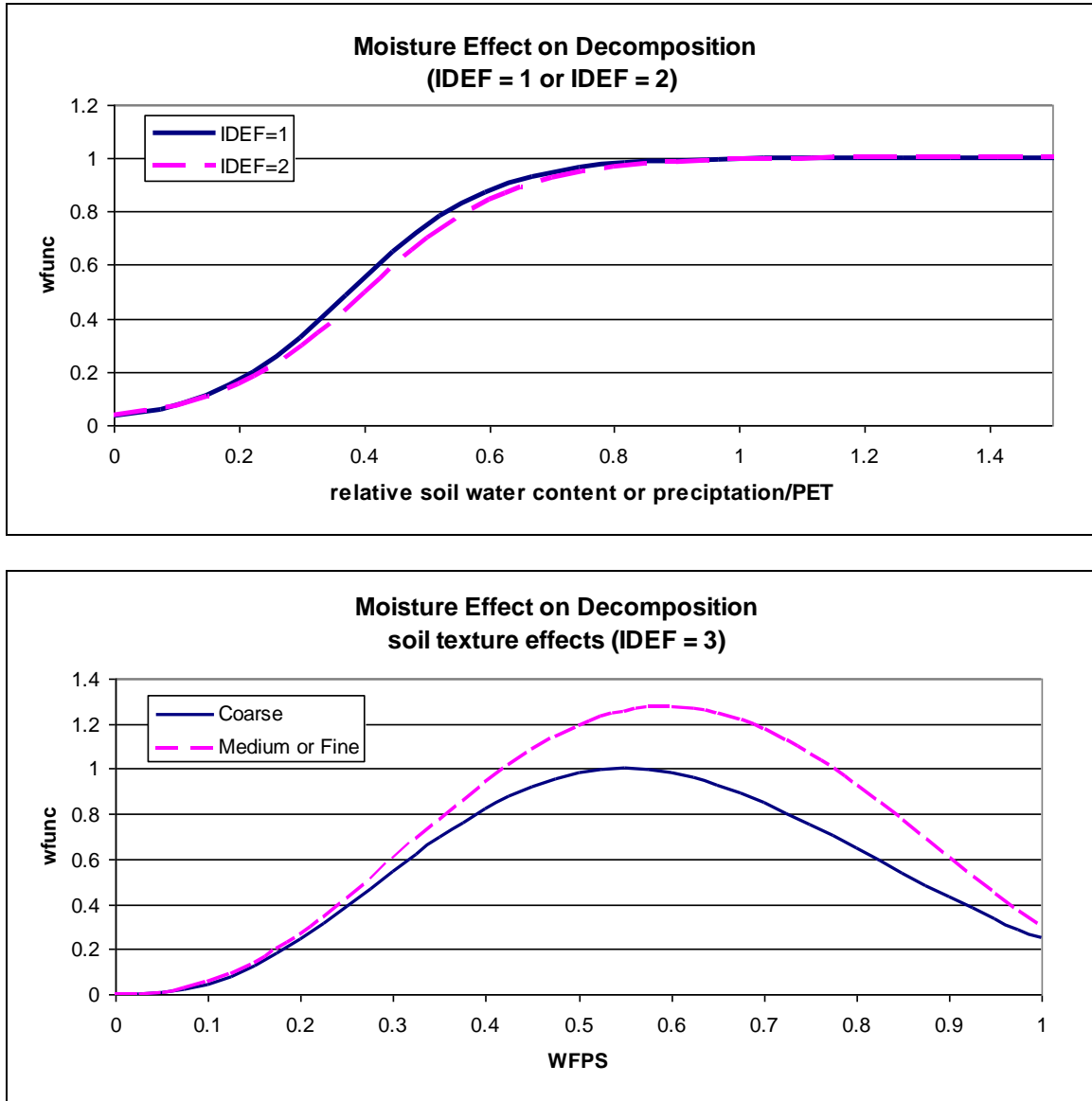
Figure WFUNC. The moisture effect on decomposition (*wfunc*): (a) When IDEF = 1 or 2. For these cases, *wfunc* strictly increases with available moisture. (b) When IDEF = 3. For this case, *wfunc* is a maximum when soil moisture is close to 50% saturated, and decreases as the soil dries or as it becomes saturated. For a given moisture content, *wfunc* is less in coarse soils compared to finer soils.

2.5.3 pH Effect on Decomposition

The pH effect on decomposition (*pHeffect*, 0– 1) depends on the soil pH (*pH*) and the dominant type of decomposer (fungi, bacteria, or a combination of both) and is calculated as

$$pHeffect = b + \frac{c}{\pi} \arctan\left(\pi d \left(pH - a\right)\right)$$

$$pHeffect = \max(pHeffect, 0.0) \tag{2.26}$$

$$pHeffect = \min(pHeffect, 1.0)$$

For *pHeff$_{fungi}$,* $a = 3.0, b = 0.5, c = 1.10, d = 0.7$
For *pHeff$_{combination}$*, $a = 4.0, b = 0.5, c = 1.10, d = 0.7$
For *pHeff$_{bacteria}$*, $a = 4.8, b = 0.5, c = 1.14, d = 0.7$

For decomposition of *metabc(*), pHeff$_{bacteria}$* is used. For decomposition of *som1c(*), som2c(*), strucc(*), wood1c, wood2c,* and *wood3c*, *pHeff$_{combination}$* is used. For decomposition of *som3c*, *pHeff$_{fungi}$* is used.
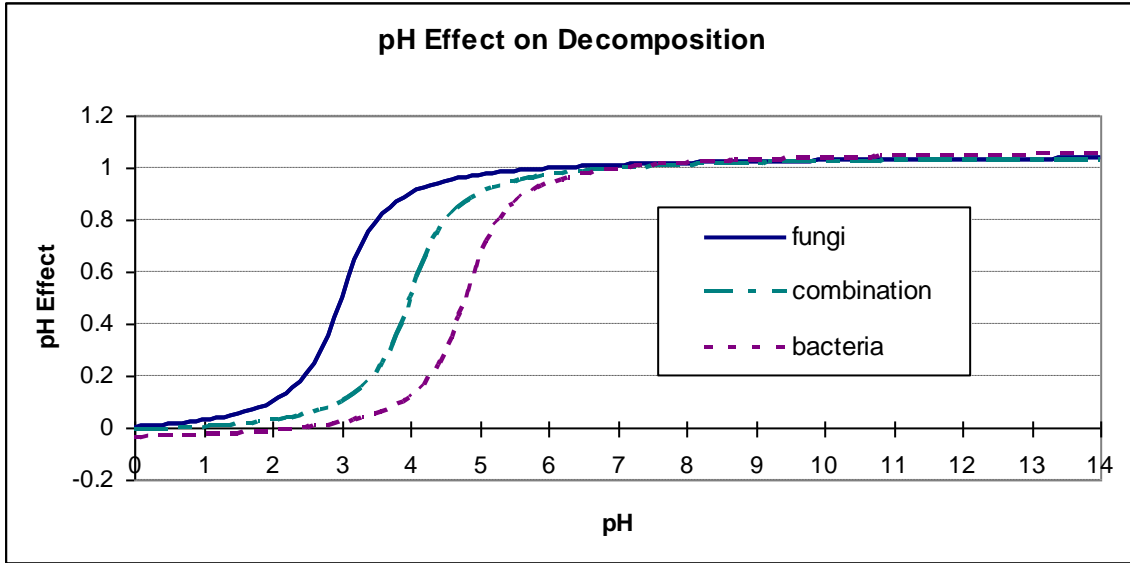
Figure PH. The three functions to determine the pH effect on decomposition vary with the type of decomposer. Minimum decomposition rates occur when the value of *pHEffect* is near zero, while the maximum rate of decomposition occurs when the value of *pHEffect* is 1.0. Decomposition at low pH is promoted by fungi, while decomposition at higher pH is it is regulated by bacteria. When pH ≥ 7.0, *pHEffect* is always 1.0.

2.5.4 Anaerobic Decomposition Factor

The anaerobic impact factor on decomposition, *anerb* where $1.0 \geq anerb \geq aneref(3)$ is calculated as

$$slope = \frac{1.0 - aneref(3)}{aneref(1) - aneref(2)} \tag{2.27}$$

$$anerb = \begin{cases} 1.0 & rprpet < aneref(1) \\ \max\left(\begin{array}{l} 1.0 + slope \times (rprpet - aneref(1)) \times (1.0 - drain), \\ aneref(3) \end{array}\right) & rprpet \geq aneref(1) \end{cases} \tag{2.28}$$

where *aneref(2)* are *fix.100* parameters, and *rprpet* is the ratio of available water to the potential evaporation rate (Eq. 2.23), *aneref(1)* is the value of *rprpet* below which there is no anaerobic impact, *aneref(2)* is used to calculate the *slope* of the impact (*aneref(2)* > *aneref(1)*), *aneref(3)* is the minimum value *anerb* (the maximum reduction in decomposition rate), and *drain* is a *fix.100* parameter that specifies the fraction of excess water lost by drainage (**Figure ANERB**).

Anaerobic Effect
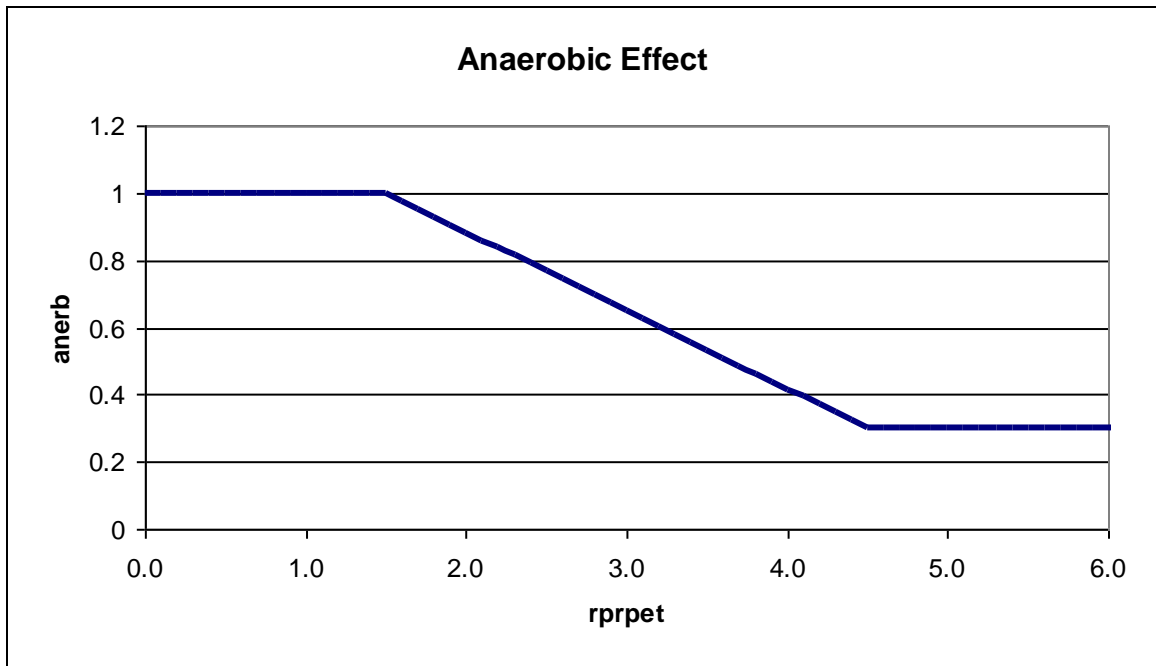
Figure ANERB. In the example graph above, *aneref(1)* = 1.5, *aneref(2)* = 3.0; *aneref(3)* = 0.3; *drain* = 0.5. When *anerb* is 1.0, there is no reduction in the decomposition rate.

2.5.5 Variable carbon to element ratios

Above ground decomposition ratio

The *agdrat* function returns the C/E ratio of material flowing into one of the *surface* soil organic matter pools. The value of *agdrat* is restricted by three variable ratio parameters, *varat(*, iel)*, and by *aminrl(iel)*, the available mineral E in top soil layer (g E m^{-2}), where *iel* is the index to element for which ratio is being computed: 1 for N, 2 for P, 3 for S (Table 2.2). The available mineral E in a layer is equal to the total mineral E in the layer except for P where some mineral P may be sorbed or occluded. The three *fix.100* parameters that restrict the value of *agdrat*, *varat(1,iel), varat(2,iel),* and *varat(3,iel),* belong to one of the following groups, depending on the destination of the organic matter flow:

varat11(1,iel) – maximum C/E ratio for material flowing into *surface* som1c
varat11(2,iel) – minimum C/E ratio for material flowing into *surface* som1c
varat11(3,iel) – amount of available mineral E that must exist or be exceeded for the minimum C/E ratio

varat21(1,iel) – maximum C/E ratio for material flowing into *surface* som2c
varat21(2,iel) – minimum C/E ratio for material flowing into *surface* som2c
varat21(3,iel) – amount of available mineral E that must exist or be exceeded for the minimum C/E ratio

$$agdrat = \begin{cases} varat(1,iel) & aminrl < 0 \\ \dfrac{1.0 - aminrl(iel)}{varat(3,iel)} \times \big(varat(1,iel) - varat(2,iel)\big) + varat(2,iel) & 0 < aminrl \leq varat(3,iel) \\ varat(2,iel) & aminrl > varat(3,iel) \end{cases}$$

(2.29)

Below ground decomposition ratio

The *bgdrat* function returns the C/E ratio of material flowing into one of the *soil* organic matter pools. The value of *bgdrat* is restricted by three variable ratio parameters, *varat(*, iel)*, and by *aminrl(iel)*, the available mineral E in top soil layer (g E m^{-2}), where *iel* is the index to element for which ratio is being computed: 1 for N, 2 for P, 3 for S (Table 2.2). The available mineral E in a layer is equal to the total mineral E in the layer except for P where some mineral P may be sorbed or occluded. The three *fix.100* parameters that restrict the value of *bgdrat, varat(1,iel), varat(2,iel),* and *varat(3,iel),* belong to one of the following groups, depending on the destination of the organic matter flow:

varat12(1,iel) – maximum C/E ratio for material flowing into *soil* som1c
varat12(2,iel) – minimum C/E ratio for material flowing into *soil* som1c
varat12(3,iel) – amount of available mineral E that must exist or be exceeded for the minimum C/E ratio

varat22(1,iel) – maximum C/E ratio for material flowing into *soil* som2c
varat22(2,iel) – minimum C/E ratio for material flowing into *soil* som2c
varat22(3,iel) – amount of available mineral E that must exist or be exceeded for the
minimum C/E ratio

varat3(1,iel) – maximum C/E ratio for material flowing into som3c (soil only)
varat3(2,iel) – minimum C/E ratio for material flowing into som3c (soil only)
varat3(3,iel) – amount of available mineral E that must exist or be exceeded for the
minimum C/E ratio

$$
bgdrat = \begin{cases} varat(1,iel) & aminrl \leq 0 \\ \dfrac{1.0 - aminrl(iel)}{varat(3,iel)} \times \big(varat(1,iel) - varat(2,iel)\big) + varat(2,iel) & 0 < aminrl < varat(3,iel) \\ varat(2,iel) & aminrl > varat(3,iel) \end{cases}
$$

$$(2.30)$$

Destination Pool	VARAT(1,N) Maximum C:N for material entering destination pool	VARAT(2,N) Minimum C:N for material entering destination pool	VARAT(3,N) *aminrl(N)* required for minimum C:N (g N m^{-2})
som1c(SRFC)	20	10	≥ 1.0
som1c(SOIL)	18	8	≥ 2.0
som2c(SRFC)	15	12	≥ 2.0
som2c(SOIL)	40	12	≥ 2.0
som3c	20	6	≥ 2.0

Table 2.2. Parameters controlling the variable C:N ratios of the destination pools.

Above or Below Ground Decomposition Ratio
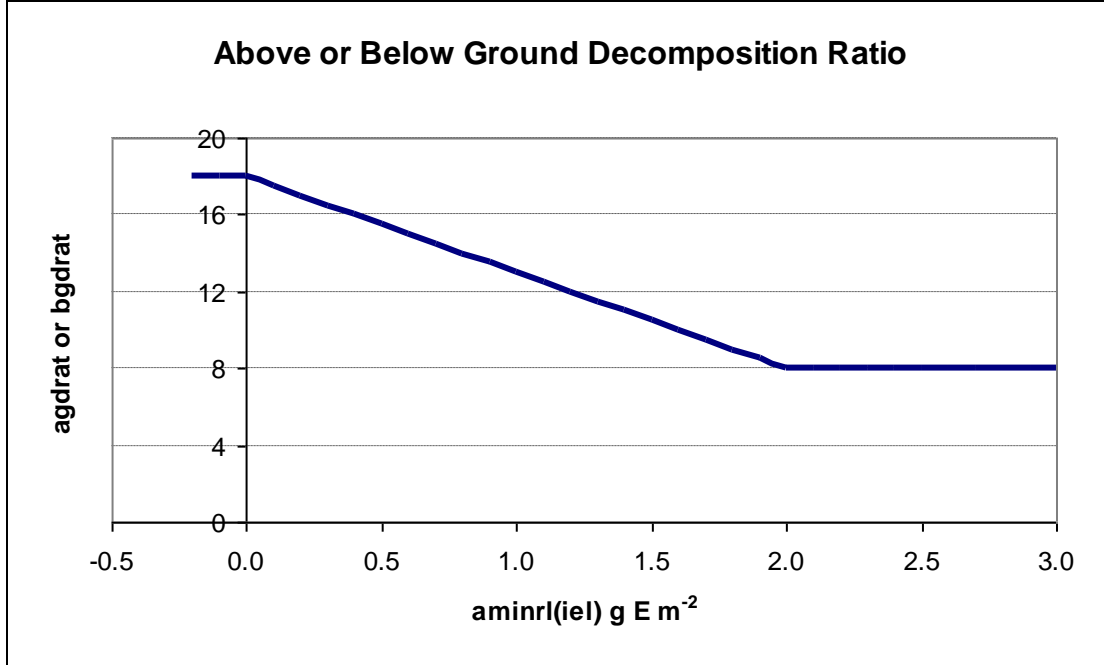
Figure DRAT. In the example above, *varat(1,iel) = 18*, *varat(2,iel) = 8*, *varat(3,iel) = 2*. In this case, when *aminrl(iel) is > 2*, the C/E ratio of decomposing material is a minimum of 8. The C/E ratio of decomposing material is greatest when available mineral E (*aminrl(iel)*) is zero.

2.6 Photodegradation of Surface Litter (photodecomp.f)

2.6.1 Standing dead plant material degrades with CO$_2$ loss but no nutrient loss

The total C flow out of *stdedc* (tcflow$_{stdedc}$, g C m^{-2}) is calculated as

$$tcflow_{stdedc} = litabs \times sradKJ \times maxphoto \qquad (2.31)$$

$$litabs = \text{line}\left(stdedc \times biocnv,\ 0.0,\ 0.0,\ bioabsorp,\ 1.0\right) \qquad (2.32)$$

$$sradKJ = srad\left(day\right) \times 86.4 \qquad (2.33)$$

where *litabs* in the litter absorption coefficient (0 – 1), *sradKJ* is the average incoming solar radiation above the plant canopy (KJ m^{-2} day^{-1}), *srad(day)* is the average incoming solar radiation above the plant canopy (W m^{-2}) , *maxphoto* is the maximum carbon loss due to photodecomposition (μg C/KJ, *sitpar.in*), *biocnv* is a factor to convert carbon to

biomass for all organic material but wood (2.5 g biomass / g C), and *bioabsorp* is the litter biomass for full absorption of solar radiation (g biomass m^{-2}, *sitepar.in*).

The CO_2 loss from *stdedc* ($co2los_{stdedc}$, g C m^{-2}) is calculated as

$$co2los_{stdedc} = tcflow_{stdedc} \times 0.48 \tag{2.34}$$

where $tcflow_{stdedc}$ is the total C flow out of standing dead pool (g C m^{-2}), Eq. 2.31). The remaining C ($tcflow_{stdedc}$ - $co2los_{stdedc}$) flows to the C source/sink with no nutrient loss.

2.6.2 Photodegradation of *strucc(SRFC)* to *metabc(SRFC)* with CO_2 loss

If $aminrl(iel) > 10^{-7}$ g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *strucc(SRFC)* is small enough to meet the required C/E of material flowing to *metabc(SRFC)* so that no immobilization occurs, then *strucc(SRFC)* can decompose.

The total C flow out of *strucc(SRFC)* ($tcflow_{strcc(SRFC)}$, g C m^{-2}) is computed as

$$tcflow_{strucc(SRFC)} = litabs \times soilsrad \times maxphoto \tag{2.35}$$

$$litabs = \text{line}\left(strucc(SRFC) \times biocnv,\ 0.0,\ 0.0,\ bioabsorp,\ 1.0\right) \tag{2.36}$$

$$soilsrad\ =\ srad\left(day\right) \times 86.4 \times \exp(-0.5 \times strlai) \tag{2.37}$$

where *soilsrad* incoming solar radiation at the bottom of the plant canopy (KJ m^{-2} day^{-1}), *litabs* is the litter absorption coefficient (0 – 1), *maxphoto* is the maximum carbon loss due to photodecomposition (µg C/KJ, *sitepar.in*), *biocnv* is a factor to convert carbon to biomass for all organic material but wood (2.5 g biomass / g C), *bioabsorp* is the litter biomass for full absorption of solar radiation (g biomass m^{-2}, *sitepar.in*), *srad(day)* is the average incoming solar radiation above the plant canopy (W m^{-2}), and *stcrlai* is the standing "crop" Leaf Area Index.

The CO_2 loss from *strucc(SRFC)* ($co2los_{strucc(SRFC)}$, g C m^{-2}) is calculated as

$$co2los_{strucc(SRFC)} = tcflow_{strucc(SRFC)} \times 0.48 \tag{2.38}$$

where $tcflow_{strucc(SRFC)}$ is the total C flow out of *strucc(SRFC)* (g C m^{-2}, Eq. 2.35).

The net carbon flow from *strucc(SRFC)* to *metabc(SRFC)* (*ctometabc1*, g C m-2) is computed as

$$ctometabc1 = tcflow_{strucc(SRFC)} - co2los_{strucc(SRFC)} \tag{2.39}$$

where $tcflow_{strucc(SRFC)}$ is the total C flow out of *strucc(SRFC)* (g C m^{-2}, Eq. 2.35),
and $co2los_{strucc(SRFC)}$ is the CO_2 loss from *strucc(SRFC)* (g C m^{-2}, Eq. 2.38).

The amount of organic E flowing from *struce(SRFC,iel)* to *metabe(SRFC, iel)*
(*eflow(iel)*, g E m^{-2}) is proportional to the total C flow out of *strucc(SRFC)*
(*tcflow_{strucc(SRFC)}* , g C m^{-2}) and is computed as

$$eflow(iel) = \frac{tcflow_{strucc(SRFC)}}{rceto1(iel)} \tag{2.40}$$

where *recto1(iel)* is the C/E ratio of the structural surface litter.

2.7 Litter Decomposition (litdec.f)

Decompose structural and metabolic material for the surface and soil. The decomposition of both structural material and dead wood (Section 2.8) requires the decomposition of lignin (**Figure DECLIG**).

Lignin Decomposition (declig)
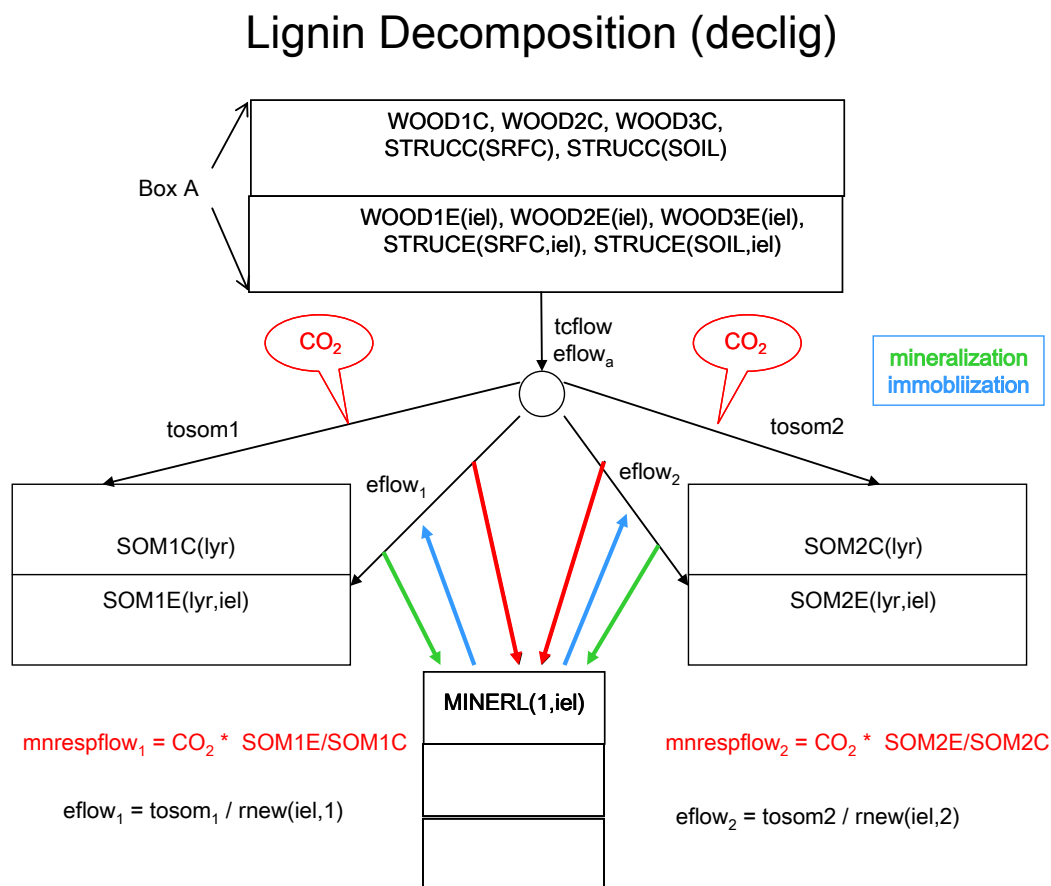
Figure DECLIG. The decomposition of lignin from structural litter (*strucc(SRFC)* or *strucc(SOIL)*)) and dead wood pools (*wood1c*, *wood2c*, or *wood3c*) to *som1c(lyr)* and *som2c(lyr),* where *lyr = SRFC* or *SOIL*. The total C flow out of Box A is *tcflow* and the flow of E out of Box A is *eflow$_a$*. The amount *tcflow* is partitioned to *som1c* and *som2c* with CO_2 loss from respiration. The amounts of N, P, and S that flow (*eflow$_1$* and *eflow$_2$*) to the corresponding *som1e* and *som2e* pools are determined by the C/E ratio required by the destination pools, (*rnew(iel,1)* and *rnew(iel,2)*. The flow of E from the source pool losses E due to the mineralization associated with respiration (*mnrespflow$_1$* and *mnrespflow$_2$*) (red arrows), then either gains E if immobilization occurs (blue arrows) or releases more E if mineralization occurs (green arrows) so that the flows are exactly equal to *eflow1* and *eflow2*. Mineralization and immobilization flows move to/from the top mineral soil layer, *minerl(1,iel)*. The associated calculations are found in declig.
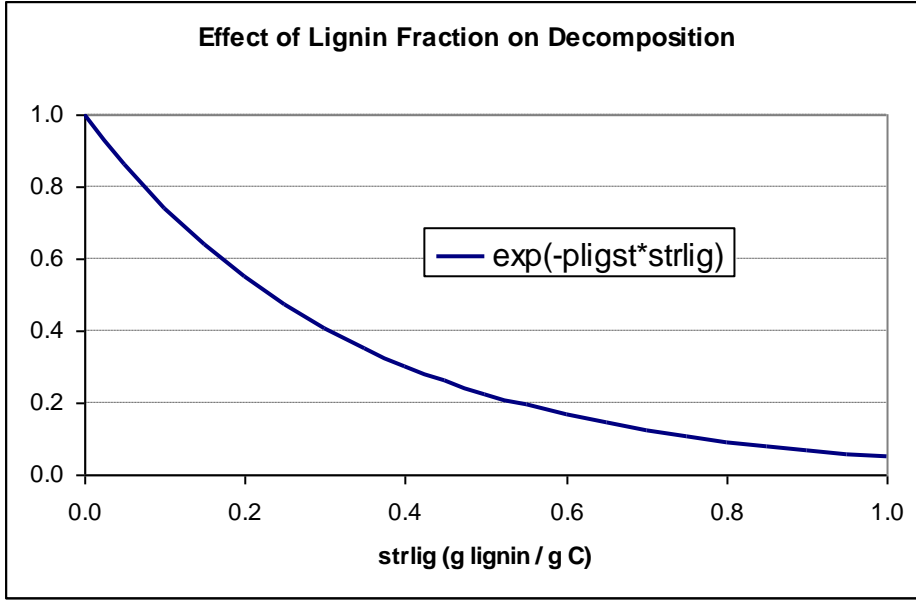
Figure LigninFrac. The effect of the lignin content of decomposing material on the rate of decomposition. As the lignin fraction of decomposition material (*strlig*, g lignin C / g C) increases, the decomposition rate of the material decreases. For this example, *pligst*, a parameter that represents the effect of lignin-to-structural-ratio on structural decomposition (*fix.100*), is 3.0.

2.7.1 Structural Litter Material

Decomposition of *strucc(SRFC)* into *som2c(SRFC)* and *som1c(SRFC)* with CO_2 loss

The total C flow out of *strucc(SRFC)* (*tcflow$_{strucc(SRFC)}$*, g C m^{-2}) is computed as

$$
\begin{aligned}
tcflow_{strucc(SRFC)} = {} & \min(strucc(SRFC), strmx(SRFC)) \\
& \times agdefac \times dec1(SRFC) \\
& \times \exp\left(-pligst(SRFC) \times strlig(SRFC)\right) \\
& \times pheff_{combination} \times dtm
\end{aligned}
\tag{2.41}
$$

where *strmx(SRFC)* is the maximum amount of surface structural that will decompose (g C m^{-2}, *fix.100*), *agdefac* is the aboveground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), *dec1(SRFC)* is the intrinsic decomposition rate of surface structural C (yr^{-1}, *fix.100*), *pligst(SRFC)* is a parameter that represents the effect of lignin-to-structural-ratio on structural decomposition (*fix.100*), *strlig(SRFC)* is the lignin content of surface structural residue (g lignin C / g C) (**Figure LigninFrac**), *pHeff$_{combination}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

Decomposition of *strucc(SRFC)* into *som2c(SRFC)*

If *aminrl(iel)* > 10^{-7} g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *strucc(SRFC)* is small enough to meet the required C/E of material flowing to *som2c(SRFC)* so that no immobilization occurs, then *strucc(SRFC)* can decompose.

The respiration associated with the C flow from *strucc(SRFC)* into *som2c(SRFC)* (*co2los$_2$*, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and the net C flow from *strucc(SRFC)* into *som2c(SRFC)* (*tosom2*, g C m^{-2}) are calculated as

$$co2los_2 = tcflow_{strucc(SRFC)} \times strlig\left(SRFC\right) \times rsplig \tag{2.42}$$

$$mnrespflow(iel) = co2los_2 \times \frac{struce\left(SRFC,iel\right)}{strucc(SRFC)} \tag{2.43}$$

$$tosom2 = tcflow_{strucc(SRFC)} \times strlig\left(SRFC\right) \times (1.0 - rsplig) \tag{2.44}$$

where *tcflow$_{strucc(SRFC)}$* is the total C flow from *strucc(SRFC)* (g C m^{-2}, Eq. 2.41), *strlig(SRFC)* (g lignin C / g C) is the lignin content of *strucc(SRFC)* and *rsplig* is the fraction of lignin flow lost as CO_2 (0 – 1, *fix.100*).

The flow of *tosom2* from *strucc(SRFC)* to *som2c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *struce(SRFC,iel)* (*eflow$_{struce(SRFC)}$*, g E m^{-2}), and the amount of E flowing into *som2e(SRFC,iel)* (*eflow$_2$*, g E m^{-2}) are calculated as

$$eflow_{struce(SRFC,iel)} = tosom2 \times \frac{struce(SRFC,iel)}{strucc(SRFC)} \tag{2.45}$$

$$eflow_2 = \frac{tosom2}{rnew\left(iel,2\right)} \tag{2.46}$$

$$mnrflow(iel) = eflow_{struce(SRFC,iel)} - eflow_2 \tag{2.47}$$

where *rnew(iel,2)* is the C/E ratio required by *som2c(SRFC)*, calculated using the *agdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel)* > *0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

Decomposition of *strucc(SRFC)* into *som1c(SRFC)*

The respiration associated with the C flow from *strucc(SRFC)* into *som1c(SRFC)* (*co2los$_1$*, g C m^{-2}) , the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from s*trucc(SRFC)* into *som1c(SRFC)* (*tosom1*, g C m^{-2}) are calculated as

$$co2los_1 = (tcflow_{strucc(SRFC)} - tosom2 - co2los_2) \times ps1co2(SRFC) \qquad (2.48)$$

$$mnrespflow(iel) = co2los_1 \times \frac{struce(SRFC,iel)}{strucc(SRFC)} \qquad (2.49)$$

$$tosom1 = (tcflow_{strucc(SRFC)} - tosom2 - co2los_2) \times (1.0 - ps1co2(SRFC)) \qquad (2.50)$$

where *tcflow$_{strucc(SRFC)}$* is the total C flow from *strucc(SRFC)* (g C m^{-2}, Eq. 2.41), *tosom2* is the C flow from *strucc(SRFC)* to *som2c(SRFC)* (g C m^{-2}, Eq. 2.44), *co2los$_2$* is the respiration loss when *strucc(SRFC)* decomposes to *som2c(SRFC)* (g C m^{-2}, Eq. 2.42), and *ps1co2(SRFC)* is a *fix.100* parameter $(0 - 1)$.

The flow of *tosom1* from *strucc(SRFC)* to *som1c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *struce(SRFC,iel) (eflow$_{struce(SRFC)}$*, g E m^{-2}), and the amount of E flowing into *som1e(SRFC,iel)* (*eflow$_1$*, g E m^{-2}) are calculated as

$$eflow_{struce(SRFC,iel)} = tosom1 \times \frac{struce(SRFC,iel)}{strucc(SRFC)} \qquad (2.51)$$

$$eflow_1 = \frac{tosom1}{rnew(iel,1)} \qquad (2.52)$$

$$mnrflow(iel) = eflow_{struce(SRFC,iel)} - eflow_1 \qquad (2.53)$$

where *rnew(iel,1)* is the C/E ratio required by *som1c(SRFC)*, calculated using the *agdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

Decomposition of *strucc(SOIL)* into *som2c(SOIL)* and *som1c(SOIL)* with CO$_2$ loss

The total C flow out of the *strucc(SOIL)* (*tcflow$_{strucc(SOIL)}$*, g C m^{-2}) is computed as

$$tcflow_{strucc(SOIL)} = \min(strucc(SOIL), strmx(SOIL))$$
$$\times bgdefac \times dec1(SOIL)$$
$$\times \exp\left(-pligst(SOIL) * strlig\left(SOIL\right)\right) \quad (2.54)$$
$$\times cltfac(4) \times anerb \times pheff_{combination} \times dtm$$

where *strmx(SOIL)* is the maximum amount of soil structural C that will decompose (g C m^{-2}, *fix.100*), *bgdefac* is the belowground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), *dec1(SOIL)* is the intrinsic decomposition rate of soil structural C (yr^{-1}, *fix.100*), *pligst(SOIL)* is a parameter that represents the effect of lignin-to-structural-ratio on structural decomposition (*fix.100*), *strlig(SOIL)* is the lignin content of soil structural residue (g lignin C / g C) (**Figure LigninFrac**), *cltfac(4)* is the cultivation factor for soil structural material (it equals clteff(4) from *cult.100* if cultivation has occurred in the past month, otherwise it equals 1.0), *anerb* is the impact of soil anaerobic conditions on decomposition (0 – 1, Eq. 2.28), *pHeff$_{combination}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

Decomposition of *strucc(SOIL)* into *som2c(SOIL)*

If *aminrl(iel)* > 10^{-7} g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *strucc(SOIL)* is small enough to meet the required C/E of material flowing to *som2c(SOIL)* so that no immobilization occurs, then *strucc(SOIL)* can decompose.

The respiration associated with the C flow from *strucc(SOIL)* into *som2c(SOIL)* (*co2los$_2$*, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and the net C flow from *strucc(SOIL)* into *som2c(SOIL)* (*tosom2*, g C m^{-2}) are calculated as

$$co2los_2 = tcflow_{strucc(SOIL)} \times strlig(SOIL) \times rsplig \quad (2.55)$$

$$mnrespflow(iel) = co2los_2 \times \frac{struce\left(SOIL, iel\right)}{strucc(SOIL)} \quad (2.56)$$

$$tosom2 = tcflow_{strucc(SOIL)} \times strlig(SOIL) \times (1.0 - rsplig) \quad (2.57)$$

where *tcflow$_{strucc(SOIL)}$* is the total C flow from *strucc(SOIL)* (g C m^{-2}, Eq. 2.54), *strlig(SOIL)* is the lignin content of *strucc(SOIL)* (g lignin C / g C), and *rsplig* is the fraction of lignin flow lost as CO$_2$ (0 – 1, *fix.100*).

The flow of *tosom2* from *strucc(SOIL)* to *som2c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *struce(SOIL,iel)* (*eflow$_{struce(SOIL)}$*, g E m^{-2}), and the amount of E flowing into *som2e(SOIL,iel)* (*eflow$_2$*, g E m^{-2}) are calculated as

$$eflow_{struce(SOIL,iel)} = tosom2 \times \frac{struce(SOIL,iel)}{strucc(SOIL)} \qquad (2.58)$$

$$eflow_2 = \frac{tosom2}{rnew(iel,2)} \qquad (2.59)$$

$$mnrflow(iel) = eflow_{struce(SOIL,iel)} - eflow_2 \qquad (2.60)$$

where *rnew(iel,2)* is the C/E ratio required by *som2c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

Decomposition of *strucc(SOIL)* into *som1c(SOIL)*

The respiration associated with the C flow from strucc(SOIL) into *som1c(SOIL)* (*co2los$_1$*, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from *strucc(SOIL)* into *som1c(SOIL)* (*tosom1*, g C m^{-2}) are calculated as

$$co2los_1 = (tcflow_{strucc(SOIL)} - tosom2 - co2los_2) \times ps1co2(SOIL) \qquad (2.61)$$

$$mnrespflow(iel) = co2los_1 \times \frac{struce(SOIL,iel)}{strucc(SOIL)} \qquad (2.62)$$

$$tosom1 = (tcflow_{strucc(SOIL)} - tosom2 - co2los_2)(1.0 - ps1co2(SOIL)) \qquad (2.63)$$

where *tcflow$_{strucc(SOIL)}$* is the total C flow from *strucc(SOIL)* (g C m^{-2}, Eq. 2.54), *tosom2* is the C flow from *strucc(SOIL)* to *som2c(SOIL)* (g C m^{-2},from Eq. 2.57), *co2los$_2$* is the respiration loss when *strucc(SOIL)* decomposes to *som2c(SOIL)* (g C m^{-2}, Eq. 2.55), and *ps1co2(SOIL)* is a *fix.100* parameter $(0 – 1)$.

The flow of *tosom1* from *strucc(SOIL)* to *som1c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *struce(SOIL,iel) (eflow$_{struce(SRFC)}$*, g E m^{-2}), and the amount of E flowing into *som1e(SOIL,iel)* (*eflow$_1$*, g E m^{-2}) are calculated as

$$eflow_{struce(SOIL,iel)} = tosom1 \times \frac{struce(SOIL,iel)}{strucc(SOIL)} \qquad (2.64)$$

$$eflow_1 = \frac{tosom1}{rnew(iel,1)} \qquad (2.65)$$

$$mnrflow(iel) = eflow_{struce(SOIL,iel)} - eflow_1 \qquad (2.66)$$

where *rnew(iel,1)* is the C/E ratio required by *som1c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

2.7.2 Metabolic Material

Metabolic Decomposition Reducer

Metabolic litter decomposes to the active soil organic matter pool. The metabolic decomposition reducer (*mdr*, 0.2 – 1.0) controls the rate that surface metabolic litter decomposes and is determined by incoming solar radiation at the bottom of the plant canopy (*soilsrad*, KJ m^{-2} day^{-1}, Eq. 2.37) ; it is calculated as

$$mdr = \begin{cases} a & soilsrad \le x_1 \\ abs\left(\dfrac{b-a}{x_2-x_1}\right)(x_2 - soilsrad) + b & x_1 < soilsrad < x_2 \\ b & soilsrad \ge x_2 \end{cases} \qquad (2.67)$$

where *a* = 1.0, *b* = 0.2, *x₁* = 0.0, and *x₂* = 30000.0 (**Figure MDR**).
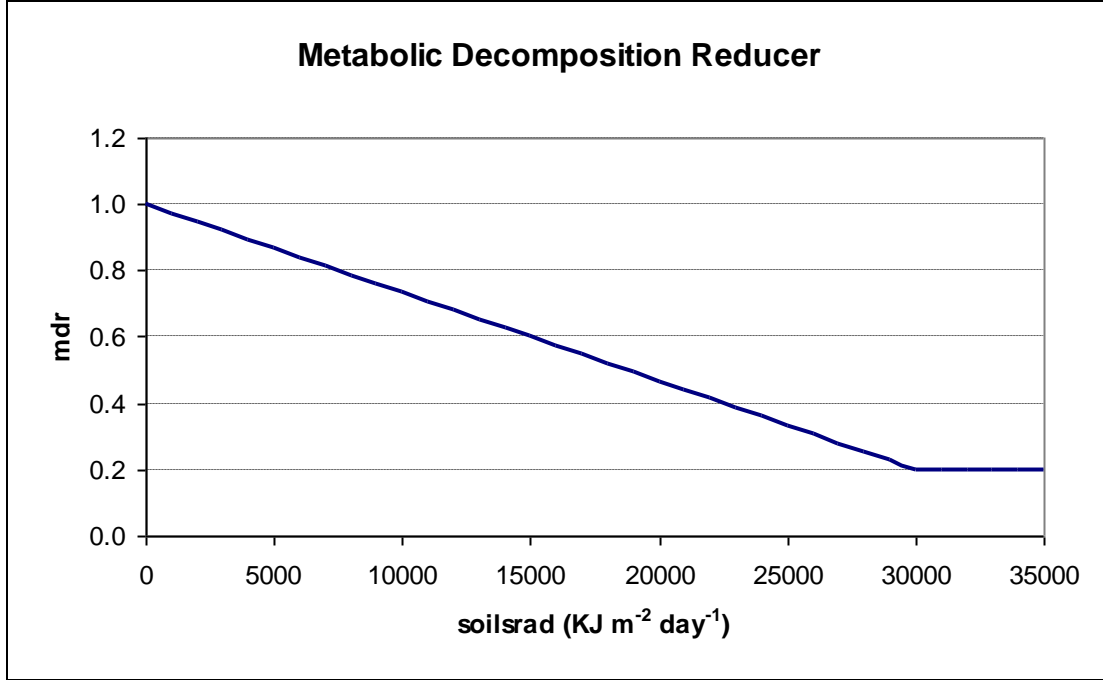
Figure MDR. Increasing soil radiation decreases the metabolic decomposition reducer (*mdr*) and therefore decreases the rate of surface metabolic litter decomposition.

Decompostion of *metabc(SRFC)* into *som1c(SRFC)* with CO_2 loss

The total C flow out of *metabc(SRFC)* ($tcflow_{metabc(SRFC)}$, g C m^{-2}) is computed as

$$tcflow_{metabc(SRFC)} = metabc(SRFC) \times agdefac \times dec2(SRFC)$$
$$\times pheff_{bacteria} \times mdr \times dtm$$

(2.68)

where *agdefac* is the aboveground decomposition factor based on water and temperature $(0 - 1$, Eq. 2.19), *dec2(SRFC)* is the intrinsic decomposition rate of surface metabolic C (yr^{-1}, *fix.100*), *pHeff$_{bacteria}$* is the pH effect on decomposition $(0 - 1$, Eq. 2.26), *mdr* is the metabolic decomposition reducer (Eq. 2.67), and *dtm* is the time step (fraction of a year, Eq. 2.2).

If *aminrl(iel)* $> 10^{-7}$ g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *metabc(SRFC)* is small enough to meet the required C/E of material flowing to *som1c(SRFC)* so that no immobilization occurs, then *metabc(SRFC)* can decompose.

The CO_2 respiration loss (*co2los*, g C m^{-2}) when *metabc(SRFC)* decomposes, the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and the net C flow from *metabc(SRFC)* into *som1c(SRFC)* (*cfmes1*, g C m^{-2}) are computed as

$$co2los = tcflow_{metabc(SRFC)} \times pmco2\left(SRFC\right) \qquad (2.69)$$

$$mnrespflow(iel) = co2los \times \frac{metabe\left(SRFC,iel\right)}{metabc(SRFC)} \qquad (2.70)$$

$$cfmes1 = tcflow_{metabc(SRFC)} \times (1.0 - pmco2(SRFC)) \qquad (2.71)$$

where *tcflow_{metabc(SRFC)}* is the total C flow from *metabc(SRFC)* to *som1c(SRFC)* (g C m^{-2}, Eq. 2.68), and *pmco2(SRFC)* is a *fix.100* parameter (0 – 1).

The flow of *cfmes1* from *metabc(SRFC)* to *som1c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *metabe(SRFC,iel)* (*eflow_{metabe(SRFC,iel)}*, g E m^{-2}), and the amount of E flowing into *som1e(SRFC,iel)* (*eflow_b*, g E m^{-2}) are calculated as

$$eflow_{metabe(SRFC,iel)} = cfmes1 \times \frac{metabe(SRFC,iel)}{metabc(SRFC)} \qquad (2.72)$$

$$eflow_b = \frac{cfmes1}{rcetob} \qquad (2.73)$$

$$mnrflow(iel) = eflow_{metabe(SRFC,iel)} - eflow_b \qquad (2.74)$$

where *rcetob* is the C/E ratio required by *som1c(SRFC)*, calculated using the a*gdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to minerl(1,iel); otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

Soil Organic Matter Nutrient Cycling

SOM1C(lyr),
SOM2C(lyr)
SOM3C,
METABC(lyr)

SOM1E(lyr,iel),
SOM2E(lyr,iel)
SOM3E(iel),
METABE(lyr,iel)

lyr=SRFC,SOIL (or 1,2)
Iel=N,P,S (or 1,2,3)

SOM Box A

tCa = total C
tEa = total E

tcflow

CO_2

cflow = tcflow – CO_2

eflow$_a$ = cflow * tEa / TCa

mnrespflow = CO_2 * tEa / tCa

immob

mnrflo

eflow$_b$ =cflow / rcetob

minerl(1,E)

minerl(2,E)

minerl(3,E)

SOM Box B

rcetob is the required C/E ratio
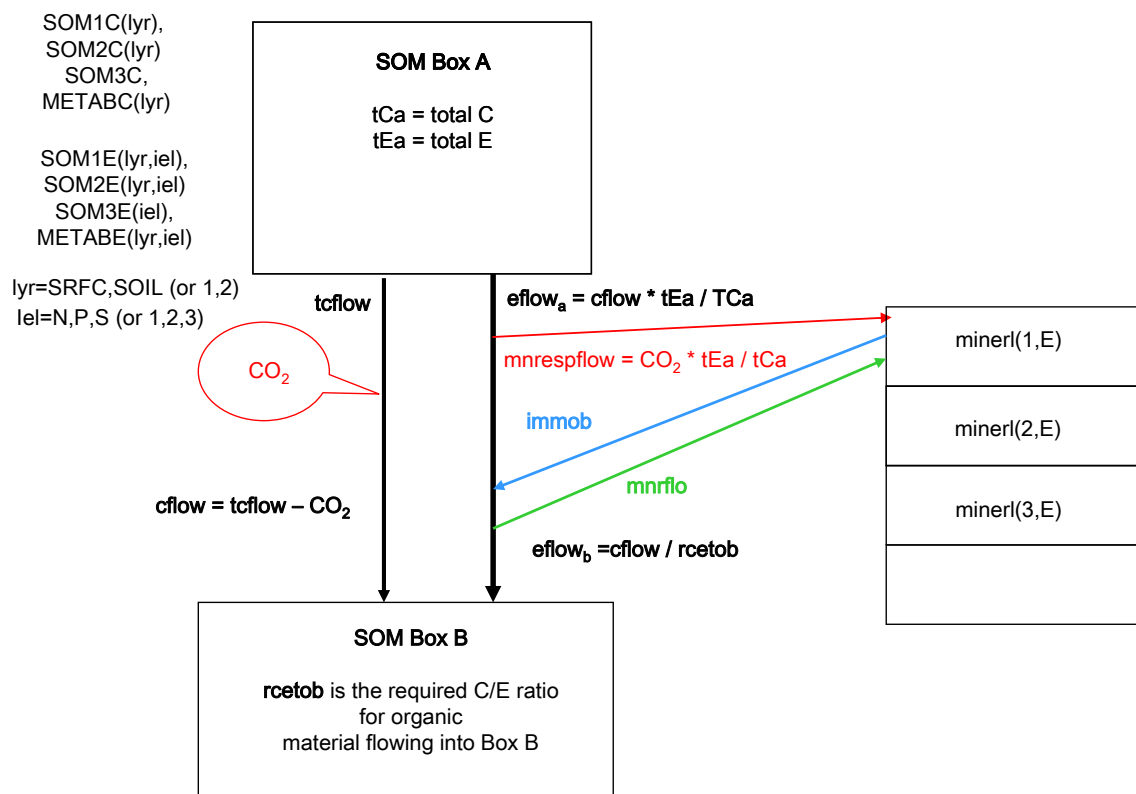for organic
material flowing into Box B

Figure FLOWS. The flow of C and E (N, P, or S) when organic matter in Box A decomposes to Box B. The C state variables represented by Box A (with **tCa** g C m^{-2}) or Box B include *som1c*, *som2c*, *som3c*, and *metabc*. The E state variables represented by Box A (with **tEa** g E m^{-2}) or Box B include *som1e*, *som2e*, *som3e*, or *metabe*. Decomposition can occur if the C/E ratio of material flowing from Box A to Box B (**tCa / tEa**) is less than **rcetob,** or the amount of available E in **minerl(1, E)** is $> 10^{-7}$ g E m^{-2}. If decomposition can occur, the amount of C flowing out of Box A (**tcflow**) minus the amount of C lost to respiration (**CO₂**, g C m^{-2}) is **cflow** (g C m^{-2}). The mineralization associated with respiration (**mnrespflow**, g E m^{-2}) (red arrow) is equal to the amount of C lost by respiration multiplied by the E/C ratio of material in Box A. The amount of E flowing out of Box A is **eflow$_a$** (g E m^{-2}), and the amount of E flowing into Box B is **eflow$_b$** (g E m^{-2}). If **eflow$_a$** – **mnrespflow** > **eflow$_b$** then mineralization (**mnrflo**) occurs (green arrow), otherwise if **eflow$_b$** > **eflow$_a$** – **mnrespflow** then immobilization (**immob**) occurs (blue arrow). The amount of **mnrflo** or **immob** is |**eflow$_a$** – **mnrespflow** – **eflow$_b$**|.

Decomposition of *metabc(SOIL)* into *som1c(SOIL)* with CO₂ loss

The total C flow out of *metabc(SOIL)* (*tcflow$_{metabc(SOIL)}$*, g C m^{-2}) is computed as

$$tcflow_{metabc(SOIL)} = metabc(SOIL) \times bgdefac \times dec2(SOIL)$$
$$\times pheff_{bacteria} \times anerb \times dtm \qquad (2.75)$$

where *bgdefac* is the belowground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), *dec2(SOIL)* is the intrinsic decomposition rate of soil metabolic C (yr^{-1}), *pHeff$_{bacteria}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), *anerb* is the impact of soil anaerobic conditions on decomposition (0 – 1, Eq. 2.28), and *dtm* is the time step (fraction of a year, Eq. 2.2).

If *aminrl(iel)* > 10^{-7} g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *metabc(SOIL)* is small enough to meet the required C/E of material flowing to *som1c(SOIL)* so that no immobilization occurs, then *metabc(SOIL)* can decompose.

The respiration loss from *metabc(SOIL)* decomposition (*co2los*, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from *metabc(SOIL)* into *som1c(SOIL)* (*cfmes1*, g C m^{-2}) are computed as

$$co2los = tcflow_{metabc(SOIL)} \times pmco2(SOIL) \qquad (2.76)$$

$$mnrespflow(iel) = co2los \times \frac{metabe(SOIL, iel)}{metabc(SOIL)} \qquad (2.77)$$

$$cfmes1 = tcflow_{metabc(SOIL)} \times (1 - pmco2(SOIL)) \qquad (2.78)$$

where *tcflow$_{metabc(SOIL)}$* is the total C flow from *metabc(SOIL)* to *som1c(SOIL)* (g C m^{-2}, Eq. 2.75), and *pmco2(SOIL)* is a *fix.100* parameter (0 – 1).

The flow of *cfmes1* from *metabc(SOIL)* to *som1c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *metabe(SOIL,iel)* (*eflow$_{metabe(SOIL,iel)}$*, g E m^{-2}), and the amount of E flowing into *som1e(SOIL,iel)* (*eflow$_b$*, g E m^{-2}) are calculated as

$$eflow_{metabe(SOIL,iel)} = cfmes1 \times \frac{metabe(SOIL, iel)}{metabc(SOIL)} \qquad (2.79)$$

$$eflow_b = \frac{cfmes1}{rcetob} \qquad (2.80)$$

$$mnrflow(iel) = eflow_{metabe(SRFC,iel)} - eflow_b \qquad (2.81)$$

where *rcetob* is the C/E ratio required by *som1c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

2.8 Dead Wood Decompostion (woodec.f)

Dead fine branches (*wood1c*), dead large wood (*wood2c*), and dead coarse roots (*wood3c*) decompose to the active and slow organic matter pools, but not to the passive pool.

2.8.1 Dead Fine Branches

The total C flow out of dead fine branches (*tcflow$_{wood1c}$*, g C m^{-2}) is calculated as

$$tcflow_{wood1c} = wood1c \times agdefac \times decw1$$
$$\times \exp\left(-pligst\left(SRFC\right) \times wdlig\left(FBRCH\right)\right) \qquad (2.82)$$
$$\times pHeff_{combination} \times dtm$$

where *wood1c* is the dead fine branch component of forest system (g C m^{-2}), *agdefac* is the aboveground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), *decw1* is the intrinsic rate of decomposition of dead fine branches (yr^{-1}, *tree.100*), *pligst(SRFC)* is a parameter that represents the effect of lignin-to-structural-ratio on structural decomposition (*fix.100*), *wdlig(FBRCH)* is the lignin fraction for fine branches (g lignin C / g C, *tree.100*) (**Figure LigninFrac**), *pHeff$_{combination}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

Decomposition of *wood1c* into *som2c(SRFC)* and *som1c(SRFC)* with CO₂ loss.

If *aminrl(iel) > 10^{-7}* g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *wood1c* is small enough to meet the required C/E of material flowing to *som1c(SRFC)* so that no immobilization occurs, then *wood1c* can decompose. If *wood1c* can't flow into *som1c(SRFC),* it can't flow into *som2c(SRFC)* either.

The respiration associated with the C flow from *wood1c* into *som2c(SRFC)* (*co2los$_2$*, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from *wood1c* into *som2c(SRFC)* (*tosom2*, g C m^{-2}) are calculated as

$$co2los_2 = tcflow_{wood1c} \times wdlig\left(FBRCH\right) \times rsplig \qquad (2.83)$$

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$$mnrespflow(iel) = co2los_2 \times \frac{wood1e(iel)}{wood1c} \qquad (2.84)$$

$$tosom2 = tcflow_{wood1c} \times wdlig(FBRCH) \times (1.0 - rsplig) \qquad (2.85)$$

where $tcflow_{wood1c}$ is the total C flow from $wood1c$ (g C m^{-2}, Eq. 2.82), $wdlig(FBRCH)$ is the lignin content of dead fine branches (g lignin C / g C, *tree.100*), and *rsplig* is the fraction of lignin flow lost as CO_2 (0 – 1, *fix.100*).

The flow of *tosom2* from *wood1c* to *som2c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *wood1e(iel)* ($eflow_{wood1e(iel)}$, g E m^{-2}), and the amount of E flowing into *som2e(SRFC,iel)* ($eflow_2$, g E m^{-2}) are calculated as

$$eflow_{wood1e(iel)} = tosom2 \times \frac{wood1e(iel)}{wood1c} \qquad (2.86)$$

$$eflow_2 = \frac{tosom2}{rnew(iel,2)} \qquad (2.87)$$

$$mnrflow(iel) = eflow_{wood1e(iel)} - eflow_2 \qquad (2.88)$$

where *rnew(iel,2)* is the C/E ratio required by *som2c(SRFC)*, calculated using the *agdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

The respiration associated with the C flow from *wood1c* into *som1c(SRFC)* ($co2los_1$, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and the net C flow from *wood1c* into *som1c(SRFC)* (*tosom1*, g C m^{-2}) are calculated as

$$co2los_1 = (tcflow_{wood1c} - tosom2 - co2los_2) \times ps1co2(SRFC) \qquad (2.89)$$

$$mnrespflow(iel) = co2los_1 \times \frac{wood1e(iel)}{wood1c} \qquad (2.90)$$

$$tosom1 = (tcflow_{wood1c} - tosom2 - co2los_2) \times (1.0 - ps1co2(SRFC)) \qquad (2.91)$$

where $tcflow_{wood1c}$ is the total C flow from *wood1c* (g C m^{-2}, Eq. 2.82), *tosom2* is the net C flow from *wood1c* into *som2c(SRFC)* (g C m^{-2}, Eq. 2.85), $co2los_2$ is the respiration

associated with the C flow from *wood1c* into *som2c(SRFC)* (g C m^{-2}, Eq. 2.83) , and *ps1co2(SRFC)* is a *fix.100* parameter $(0 - 1)$.

The flow of *tosom1* from *wood1c* to *som1c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *wood1e(iel)* (*eflow$_{wood1e(iel)}$*, g E m^{-2}), and the amount of E flowing into *som1e(SRFC,iel)* (*eflow$_1$*, g E m^{-2}) are calculated as

$$eflow_{wood1e(iel)} = tosom1 \times \frac{wood1e(iel)}{wood1c} \tag{2.92}$$

$$eflow_1 = \frac{tosom1}{rnew(iel,1)} \tag{2.93}$$

$$mnrflow(iel) = eflow_{wood1e(iel)} - eflow_1 \tag{2.94}$$

where *rnew(iel,1)* is the C/E ratio required by *som1c(SRFC)*, calculated using the *agdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

2.8.2 Large Dead Wood

The total C flow out of dead large wood (*tcflow$_{wood2c}$*, g C m^{-2}) is computed as

$$\begin{aligned} tcflow_{wood2c} &= wood2c \times agdefac \times decw2 \\ &\times \exp\left(-pligst(SRFC) \times wdlig(LWOOD)\right) \\ &\times pHeff_{combination} \times dtm \end{aligned} \tag{2.95}$$

where *wood2c* is the dead large wood component of forest system (g C m^{-2}), *agdefac* is the aboveground decomposition factor based on water and temperature $(0 - 1,$ Eq. 2.19), *decw2* is the intrinsic rate of decomposition of dead large wood (yr^{-1}, *tree.100*), *pligst(SRFC)* is the *fix.100* parameter that represents the effect of lignin-to-structural-ratio on structural decomposition, *wdlig(LWOOD)* is the lignin fraction for large wood (g lignin C / g C, *tree.100*) (**Figure LigninFrac**), *pHeff$_{combination}$* is the pH effect on decomposition $(0 - 1,$ Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

Decomposition of *wood2c* into *som2c(SRFC)* and *som1c(SRFC)* with CO$_2$ loss.

If *aminrl(iel) > 10^{-7}* g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *wood2c* is small enough to meet the required C/E of material flowing to *som1c(SRFC)* so that no immobilization occurs, then *wood2c* can decompose. If *wood1c* can't flow into *som1c(SRFC)*, it can't flow into *som2c(SRFC)* either.

The respiration associated with the C flow from *wood2c* into *som2c(SRFC)* ($co2los_2$, g C m^{-2}) , the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from *wood2c* into *som2c(SRFC)* (*tosom2*, g C m^{-2}) are calculated as

$$co2los_2 = tcflow_{wood2c} \times wdlig\left(LWOOD\right) \times rsplig \tag{2.96}$$

$$mnrespflow(iel) = co2los_2 \times \frac{wood2e\left(iel\right)}{wood2c} \tag{2.97}$$

$$tosom2 = tcflow_{wood2c} \times wdlig\left(LWOOD\right) \times (1.0 - rsplig) \tag{2.98}$$

where *tcflow$_{wood2c}$* is the total C flow from *wood2c* (g C m^{-2}, Eq. 2.95), *wdlig(LWOOD)* is the lignin content of dead large wood (g lignin C / g C, *tree.100*), and *rsplig* is the fraction of lignin flow lost as CO_2 (0 – 1, *fix.100*).

The flow of *tosom2* from *wood2c* to *som2c(SRFC)* is partitioned by isotope (csched). The amount of E flowing out of *wood2e(iel)* (*eflow$_{wood2e(iel)}$*, g E m^{-2}), and the amount of E flowing into *som2e(SRFC,iel)* (*eflow$_2$*, g E m^{-2}) are calculated as

$$eflow_{wood2e(iel)} = tosom2 \times \frac{wood2e(iel)}{wood2c} \tag{2.99}$$

$$eflow_2 = \frac{tosom2}{rnew\left(iel,2\right)} \tag{2.100}$$

$$mnrflow(iel) = eflow_{wood2e(iel)} - eflow_2 \tag{2.101}$$

where *rnew(iel,2)* is the C/E ratio required by *som2c(SRFC)*, calculated using the *agdrat* function (Eq. 2.29), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

The respiration associated with the C flow from *wood2c* into *som1c(SRFC)* ($co2los_1$, g C m^{-2}), the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and the net C flow from *wood2c* into *som1c(SRFC)* (*tosom1*, g C m^{-2}) are calculated as

$$co2los_1 = (tcflow_{wood2c} - tosom2 - co2los_2) \times ps1co2\left(SRFC\right) \tag{2.102}$$

$$mnrespflow(iel) = co2los_1 \times \frac{wood2e(iel)}{wood2c} \tag{2.103}$$

$$tosom1 = (tcflow - tosom2 - co2los_2) \times (1.0 - ps1co2(SRFC)) \tag{2.104}$$

where $tcflow_{wood2c}$ is the total C flow from $wood2c$ (g C m^{-2}, Eq. 2.95), $tosom2$ is the net C flow from $wood2c$ into $som2c(SRFC)$ (g C m^{-2}, Eq. 2.98), $co2los_2$ is the associated with the C flow from $wood2c$ into $som2c(SRFC)$ (g C m^{-2}, Eq. 2.96), and $ps1co2(SRFC)$ is a $fix.100$ parameter $(0 - 1)$.

The flow of $tosom1$ from $wood2c$ to $som1c(SRFC)$ is partitioned by isotope (csched). The amount of E flowing out of $wood2e(iel)$ ($eflow_{wood2e(iel)}$, g E m^{-2}), and the amount of E flowing into $som1e(SRFC,iel)$ ($eflow_1$, g E m^{-2}) are calculated as

$$eflow_{wood2e(iel)} = tosom1 \times \frac{wood2e(iel)}{wood2c} \tag{2.105}$$

$$eflow_1 = \frac{tosom1}{rnew(iel,1)} \tag{2.106}$$

$$mnrflow(iel) = eflow_{wood2e(iel)} - eflow_1 \tag{2.107}$$

where $rnew(iel,1)$ is the C/E ratio required by $som1c(SRFC)$, calculated using the $agdrat$ function (Eq. 2.29), and $mnrflow(iel)$ (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If $mnrflow(iel) > 0$, net mineralization occurs and $mnrflow(iel)$ is added to $minerl(1,iel)$; otherwise, immobilization occurs and $mnrflow(iel)$ is removed from $minerl(1,iel)$.

2.8.3 Dead Coarse Roots

The total C flow out of dead coarse roots ($tcflow_{wood3c}$, g C m^{-2}) is calculated as

$$\begin{aligned}
tcflow_{wood3c} = \ &wood3c \times bgdefac \times decw3 \\
&\times \exp\left(-pligst(SOIL) \times wdlig(CROOT)\right) \\
&\times anerb \times pHeff_{combination} \times dtm
\end{aligned} \tag{2.108}$$

where $wood3c$ is the dead coarse root component of forest system (g C m^{-2}), $bgdefac$ is the belowground decomposition factor based on water and temperature (0– 1, Eq. 2.19), $decw3$ is the intrinsic rate of decomposition of dead coarse roots (yr^{-1}, $tree.100$), $pligst(SOIL)$ is a parameter that represents the effect of lignin-to-structural-ratio on structural decomposition ($fix.100$), $wdlig(CROOT)$ is the lignin fraction for coarse roots (g lignin C / g C, $tree.100$) (**Figure LigninFrac**), $anerb$ is the impact of soil anaerobic

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conditions on decomposition (0 – 1, Eq. 2.28), $pHeff_{combination}$ is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

Decomposition of *wood3c* into *som2c(SOIL)* and *som1c(SOIL)* with CO₂ loss.

If $aminrl(iel) > 10^{-7}$ g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *wood3c* is small enough to meet the required C/E of material flowing to *som1c(SOIL)* so that no immobilization occurs, then *wood3c* can decompose. If *wood1c* can't flow into *som1c(SOIL)*, it can't flow into *som2c(SOIL)* either.

The respiration associated with the C flow from *wood3c* into *som2c(SOIL)* ($co2los_2$, g C m^{-2}) , the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and the net C flow from *wood3c* into *som2c(SOIL)* (*tosom2*, g C m^{-2}) are calculated as

$$co2los_2 = tcflow_{wood3c} \times wdlig(CROOT) \times rsplig \qquad (2.109)$$

$$mnrespflow(iel) = co2los_2 \times \frac{wood3e(iel)}{wood3c} \qquad (2.110)$$

$$tosom2 = tcflow_{CROOT} \times wdlig(CROOT) \times (1.0 - rsplig) \qquad (2.111)$$

where $tcflow_{wood3c}$ is the total C flow from *wood3c* (g C m^{-2}, Eq. 2.108), *wdlig(CROOT)* is the lignin content of *wood3c* (g lignin C / g C, *tree.100*), and *rsplig* is the fraction of lignin flow lost as CO₂ (0 – 1, *fix.100*).

The flow of *tosom2* from *wood3c* to *som2c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *wood3e(iel)* ($eflow_{wood3e(iel)}$, g E m^{-2}), and the amount of E flowing into *som2e(SOIL,iel)* ($eflow_2$, g E m^{-2}) are calculated as

$$eflow_{wood3e(iel)} = tosom2 \times \frac{wood3e(iel)}{wood3c} \qquad (2.112)$$

$$eflow_2 = \frac{tosom2}{rnew(iel,2)} \qquad (2.113)$$

$$mnrflow(iel) = eflow_{wood3e(iel)} - eflow_2 \qquad (2.114)$$

where *rnew(iel,2)* is the C/E ratio required by *som2c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is

added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

The respiration associated with the C flow from *wood3c* into *som1c(SOIL)* (*co2los₁*, g C m⁻²), the mineralization of element *iel* (*mnrespflow(iel)*, g E m⁻²) associated with respiration, and the net C flow from *wood3c* into *som1c(SOIL)* (*tosom1*, g C m⁻²) are calculated as

$$co2los_1 = (tcflow_{wood3c} - tosom2 - co2los_2) \times ps1co2(SOIL) \qquad (2.115)$$

$$mnrespflow(iel) = co2los_1 \times \frac{wood3e(iel)}{wood3c} \qquad (2.116)$$

$$tosom1 = (tcflow_{CROOT} - tosom2 - co2los_2) \times (1.0 - ps1co2(SOIL)) \qquad (2.117)$$

where *tcflow$_{wood3c}$* is the total C flow from *wood3c* (g C m-2, Eq. 2.108), *tosom2* is net C flow from *wood3c* into *som2c(SOIL)* (g C m⁻²), Eq. 2.111), *co2los₂* is the respiration associated with the C flow from *wood3c* into *som2c(SOIL)* (g C m-2, Eq. 2.109), and *ps1co2(SOIL)* is a *fix.100* parameter (0 – 1).

The flow of *tosom1* from *wood3c* to *som1c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *wood3e(iel)* (*eflow$_{wood3e(iel)}$*, g E m⁻²), and the amount of E flowing into *som1e(SOIL,iel)* (*eflow₁*, g E m⁻²) are calculated as

$$eflow_{wood3e(iel)} = tosom1 \times \frac{wood3e(iel)}{wood3c} \qquad (2.118)$$

$$eflow_1 = \frac{tosom1}{rnew(iel,1)} \qquad (2.119)$$

$$mnrflow(iel) = eflow_{wood3e(iel)} - eflow_1 \qquad (2.120)$$

where *rnew(iel,1)* is the C/E ratio required by *som1c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m⁻²) is the net mineralization or immobilization (**Figure DECLIG**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

2.9 Soil Organic Matter Decomposition (somdec.f).

The somdec subroutine calculates the decomposition of *som1c(SRFC), som1c(SOIL), som2c(SRFC), som2c(SOIL)*, and *som3c* (**Figure DecompC**).

2.9.1 Decomposition of *som1c(SRFC)* to *som2c(SRFC)* with CO_2 loss

The microbial turnover increase (*mti,* $1.0 - 5.0$) regulates the decomposition of *som1c(SRFC)* and is based on incoming solar radiation at the bottom of the plant canopy (*soilsrad*, KJ day^{-1}, Eq. 2.37) . It is calculated as

$$mti = \begin{cases} a & soilsrad \leq x_1 \\ \left(\dfrac{b-a}{x_2 - x_1} \right)(soilsrad - x_1) + a & x_1 < soilsrad < x_2 \\ b & soilsrad \geq x_2 \end{cases} \qquad (2.121)$$

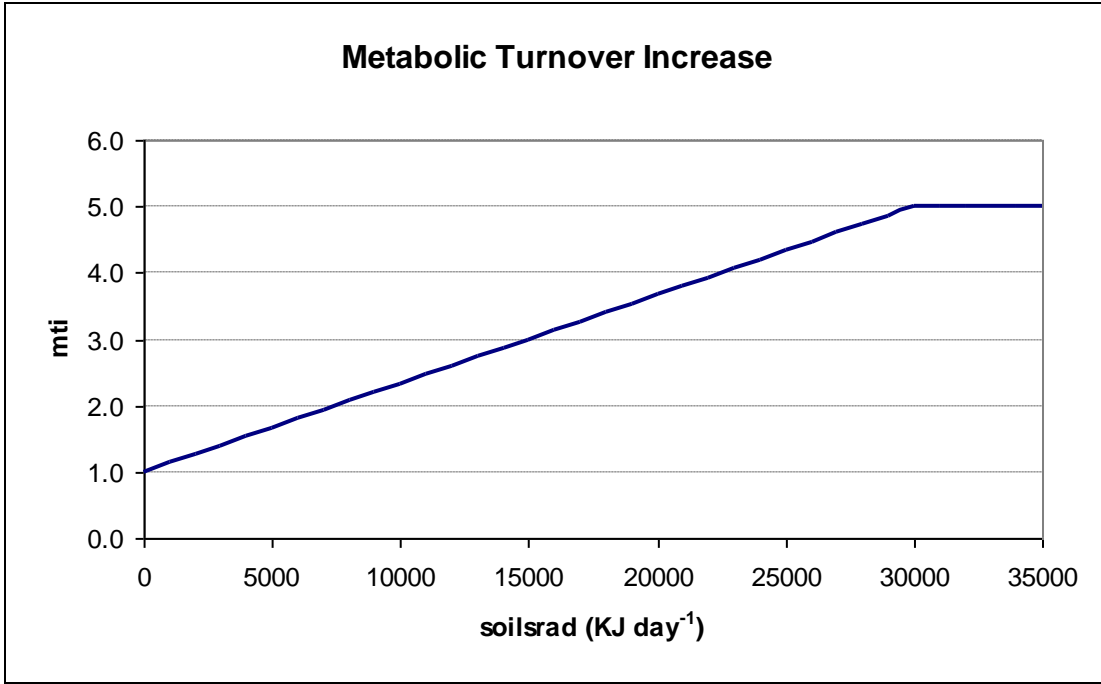where $a = 1.0$, $b = 5.0$, $x_1 = 0.0$, and $x_2 = 30000.0$.

Figure MTI. The metabolic turnover increase (*mti*) effects the rate of *som1c(SRFC)* decomposition and increases with solar radiation reaching the soil surface (*soilsrad*).

The total C flow out of *som1c(SRFC)* ($tcflow_{som1c(SRFC)}$, g C m^{-2}) is calculated as

$$tcflow_{som1c(SRFC)} = som1c(SRFC) \times agdefac \times dec3(SRFC)$$
$$\times pHeff_{combination} \times mti \times dtm \qquad (2.122)$$

where *agdefac* is the aboveground decomposition factor based on water and temperature
$(0 – 1$, Eq. 2.19), *dec3(SRFC)* is the intrinsic decomposition rate of surface microbes (yr⁻¹, *fix.100*), *pHeff_{combination}* is the pH effect on decomposition $(0 – 1$, Eq. 2.26*), mti* is the
microbial turnover increase due to solar radiation (Eq. 2.121), and *dtm* is the time step
(fraction of a year, Eq. 2.2).

If *aminrl(iel)* > 10^{-7} g E m⁻² for each mineral (N, P, S) being simulated, or if the
C/E ratio of *som1c(SRFC)* is small enough to meet the required C/E of material flowing
to *som2c(SRFC)* so that no immobilization occurs, then *som1c(SRFC)* can decompose.

The respiration associated with the C flow from *som1c(SRFC)* (*co2los*, g C m⁻²),
the mineralization of element *iel* (*mnrespflow(iel),* g E m⁻²) associated with respiration,
and the net C flow from *som1c(SRFC)* to *som2c(SRFC)* (*cfsfs2*, g C m⁻²) are calculated as

$$co2los = tcflow_{som1c(SRFC)} \times p1co2(SRFC) \qquad (2.123)$$

$$mnrespflow(iel) = co2los \times \frac{som1e(SRFC,iel)}{som1c(SRFC)} \qquad (2.124)$$

$$cfsfs2 = tcflow_{som1c(SRFC)} \times (1 - p1co2(SRFC)) \qquad (2.125)$$

where *tcflow_{som1c(SRFC)}* is the total C flow out of *som1c(SRFC)* (g C m⁻², Eq. 2.122),
p1co2(SRFC) is equal to *p1co2a(SRFC),* a *fix.100* intercept parameter which controls
flow from soil organic matter with fast turnover to CO_2 (fraction of carbon lost to CO_2
when there is no sand in the soil) $(0 – 1)$.

The flow of *cfsfs2* to *som2c(SRFC)* is partitioned by isotope (csched). The amount
of E flowing out of *som1e(SRFC,iel) (eflow_{som1e(SRFC,iel)}*, g E m⁻²), and the amount of E
flowing into *som2e(SRFC,iel) (eflow_b*, g E m⁻²) are calculated as

$$eflow_{som1e(SRFC,iel)} = tcflow_{som1c(SRFC)} \times \frac{som1e(SRFC,iel)}{som1c(SRFC)} \qquad (2.126)$$

$$eflow_b = \frac{cfsfs2}{rcetob} \qquad (2.127)$$

$$mnrflow(iel) = eflow_{som1e(SRFC,iel)} - eflow_b \qquad (2.128)$$

where *rcetob* is the C/E ratio required by *som2c(SRFC)*, calculated using the a*gdrat*
function (Eq. 2.29), and *mnrflow(iel)* (g E m⁻²) is the net mineralization or immobilization
(**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is
added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed
from *minerl(1,iel).*

2.9.2 Decomposition of *som1c(SOIL)* to *som2c(SOIL)* and *som3c* with CO₂ loss and possible leaching of organics

If *aminrl(iel)* > 10^{-7} g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *som1c(SOIL)* is small enough to meet the required C/E of material flowing to *som2c(SOIL)* so that no immobilization occurs, then *som1c(SOIL)* can decompose. If *som1c(SOIL)* can't flow into *som2c(SOIL)*, it can't flow into *som3c* either.

The total C flow out of *som1c(SOIL)* (*tcflow$_{som1c(SOIL)}$*, g C m^{-2}) is calculated as

$$tcflow_{som1c(SOIL)} = som1c(SOIL) \times bgdefac \times dec3(SOIL) \times cltfac(1)$$
$$\times eftext \times anerb \times pHeff_{bacteria} \times dtm \tag{2.129}$$

$$eftext = peftxa + peftxb \times sand \tag{2.130}$$

where *bgdefac* is the belowground decomposition factor based on water and temperature (0– 1, Eq. 2.19), *dec3(SOIL)* is the intrinsic decomposition rate of soil microbes (yr^{-1}, *fix.100*), *cltfac(1)* is the cultivation factor for *som1c* (it equals *clteff(1)* from *cult.100* if cultivation has occurred in the past month, otherwise it equals 1.0), *eftext* is the effect of soil texture on the soil microbe decomposition rate (0 – 1), *anerb* is the impact of soil anaerobic conditions on decomposition (0 – 1, Eq. 2.28), *pHeff$_{bacteria}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2). The value of *eftext* increases with the fraction of *sand* in mineral soil and is modified by the *fix.100* parameters, *peftxa* and *peftxb*.

The respiration loss when *som1c(SOIL)* decomposes (*co2los*, g C m^{-2}), and the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration are computed as

$$co2los = tcflow_{som1c(SOIL)} \times p1co2(SOIL) \tag{2.131}$$

$$mnrespflow(iel) = co2los \times \frac{som1e(SOIL,iel)}{som1c(SOIL)} \tag{2.132}$$

$$p1co2(SOIL) = p1co2a(SOIL) + p1co2b(SOIL) \times sand \tag{2.133}$$

where *tcflow$_{som1c(SOIL)}$* is the total C flow out of *som1c(SOIL)* (g C m^{-2}, Eq. 2.129), *p1co2(SOIL)* is computed from two *fix.100* parameters, *p1co2a(SOIL)* and *p1co2b(SOIL)* and the *sand* fraction of mineral soil (0 – 1).

Decomposition of *som1c(SOIL)* to *som3c*

The total C flow from *som1c(SOIL)* to *som3c* (*cfs1s3*, g C m^{-2}) is a function of clay content and computed as

$$cfs1s3 = tcflow_{som1c(SOIL)} \times fps1s3 \times \left(1.0 + animpt \times \left(1.0 - anerb\right)\right) \tag{2.134}$$

$$fps1s3 = ps1s3(1) + ps1s3(2) \times clay \tag{2.135}$$

where $tcflow_{som1c(SOIL)}$ is the total C flow out of $som1c(SOIL)$ (g C m^{-2}, Eq. 2.129), $fps1s3$ is the impact of the soil clay content on the flow $(0-1)$, $animpt$ is a slope term used to vary the impact of soil anaerobic conditions on decomposition flows to the passive soil organic matter pool (*fix.100* parameter), and $anerb$ is the anaerobic effect $(0-1$, Eq. 2.28). The value of *fps1s3* increases with the *clay* fraction of mineral soil $(0-1)$, and is modified by the *fix.100* parameters, *ps1s3(1)* and *ps1s3(2)*. There is no microbial respiration associated with this flow since the flow into *som3c* is due to physical protection of organic matter by clay, and is not a biotic process (?).

The flow of *cfs1s3* from *som1c(SOIL)* to *som3c* is partitioned by isotope (csched). The amount of E flowing out of *som1e(SOIL,iel)* ($eflow_{som1e(SOIL,iel)}$, g E m^{-2}), and the amount of E flowing into *som3e(iel)* ($eflow_b$, g E m^{-2}) are calculated as

$$eflow_{som1e(SOIL,iel)} = cfs1s3 \times \frac{som1e(SOIL,iel)}{som1c(SOIL)} \tag{2.136}$$

$$eflow_b = \frac{cfs1s3}{rcetob} \tag{2.137}$$

$$mnrflow(iel) = eflow_{som1e(SOIL,iel)} - eflow_b \tag{2.138}$$

where *rcetob* is the C/E ratio required by *som3c*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

Leaching of Organics

Leaching of organics only occurs when the water flow out of Century soil layer 2 (*amovdly(2)*, cm day^{-1}) and reaches a maximum once *amovdly(2)* exceeds a critical value, *omlech(3)*. Organic C leaching (*cleach*, g C m^{-2}) is based on the leaching intensity (*linten*, $0-1$) and the effect of soil texture on organic leaching (*orglch,* $0-1$) and is calculated as

$$cleach = tcflow_{som1c(SOIL)} \times orglch \times linten \tag{2.139}$$

$$orglch = omlech(1) + omlech(2) \times sand \tag{2.140}$$

$$linten = \min\left(1.0 - \frac{\left(omlech(3) - amovdly(2)\right)}{omlech(3)}, \ 1.0\right) \qquad (2.141)$$

where *sand* is the fraction of sand in mineral soil $(0 - 1)$, *omlech(1)*, *omlech(2)*, and *omlech(3)* are *fix.100* parameters, $tcflow_{som1c(SOIL)}$ is total C flow from *som1c(SOIL)* (g C m^{-2}, Eq. 2.129). The value of *orglch* increases with the sand content of soil.

The leaching of organic N, P, and S, (*orgEflow(iel)*, g E m^{-2}) is computed as

$$orgEflow(iel) = \frac{cleach}{rce(iel)} \qquad (2.142)$$

$$rce(iel) = \begin{cases} 2.0 \times \dfrac{som1c(SOIL)}{som1e(SOIL, iel)} & iel = N, \ S \\[4mm] 35.0 \times \dfrac{som1c(SOIL)}{som1e(SOIL, iel)} & iel = P \end{cases} \qquad (2.143)$$

where *cleach* is the amount of organic C leaching (g C m^{-2}, Eq. 2.139), and *rce(iel)* is the ratio of organic C to organic N, P, or S.

Decomposition of *som1c(SOIL)* to *som2c(SOIL)*

The flow of C from *som1c(SOIL)* to *som2c(SOIL)* (*cfs1s2*, g C m^{-2}) is computed as

$$cfs1s2 = tcflow_{som1c(SOIL)} - co2los - cfs1s3 - cleach \qquad (2.144)$$

where $tcflow_{som1c(SOIL)}$ is the total C flow out of *som1c(SOIL)* (g C m^{-2}, Eq. 2.129), *co2los* is the respiration loss when *som1c(SOIL)* decomposes (g C m^{-2}, Eq. 2.131), *cfs1s3* is amount of C flow from *som1c(SOIL)* to *som3c* (g C m^{-2}, Eq. 2.134), and *cleach* is the amount of organic C leaching (g C m^{-2}, Eq. 2.139).

The flow of *cfs1s2* from *som1c(SOIL)* to *som2c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *som1e(SOIL,iel)* (*eflow$_{som1e(SOIL,iel)}$*, g E m^{-2}), and the amount of E flowing into *som2e(SOIL, iel)* (*eflow$_b$*, g E m^{-2}) are calculated as

$$eflow_{som1e(SOIL,iel)} = cfs1s2 \times \frac{som1e(SOIL, iel)}{som1c(SOIL)} \qquad (2.145)$$

$$eflow_b = \frac{cfs1s2}{rcetob} \tag{2.146}$$

$$mnrflow(iel) = eflow_{som1e(SOIL,iel)} - eflow_b \tag{2.147}$$

where *rcetob* is the C/E ratio required by *som2c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

2.9.3 Decomposition of *som2c(SOIL)* into *som1c(SOIL)* and *som3c* with CO$_2$ loss

If *aminrl(iel) > 10^{-7}* g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *som2c(SOIL)* is small enough to meet the required C/E of material flowing to *som1c(SOIL)* so that no immobilization occurs, then *som2c(SOIL)* can decompose. If *som2c(SOIL)* can't flow into *som1c(SOIL)*, it can't flow into *som3c* either.

The total C flow out of *som2c(SOIL)* (*tcflow$_{som2c(SOIL)}$*, g C m^{-2}) is computed as

$$tcflow_{som2c(SOIL)} = som2c(SOIL) \times bgdefac \times dec5(SOIL) \times cltfac(2)$$
$$\times anerb \times pHeff_{combination} \times dtm \tag{2.148}$$

where *bgdefac* is the belowground decomposition factor based on water and temperature (0–1, Eq. 2.19), *dec5(SOIL)* is the intrinsic decomposition rate of *som2c(SOIL)* (yr^{-1}, *fix.100*), *cltfac(2)* is the cultivation factor for *som2c(SOIL)* (it equals *clteff(2)* from *cult.100* if cultivation has occurred in the past month, otherwise it equals 1.0), *anerb* is the impact of soil anaerobic conditions on decomposition (0 – 1, Eq. 2.28), *pHeff$_{combination}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

The respiration associated with the C flow from *som2c(SOIL)* (*co2los*, g C m^{-2}), and the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration are calculated as

$$co2los = tcflow_{som2c(SOIL)} \times p2co2(SOIL) \tag{2.149}$$

$$mnrespflow(iel) = co2los \times \frac{som2e(SOIL,iel)}{som2c(SOIL)} \tag{2.150}$$

where *tcflow$_{som2c(SOIL)}$* is the total C flow out of *som2c(SOIL)* (g C m^{-2}, Eq. 2.148), and *p2co2(SOIL)* is a *fix.100* parameter.

Decomposition of *som2c(SOIL)* to *som3c*

The net C flow from *som2c(SOIL)* to *som3c* (*cfs2s3*, g C m^{-2}) is a function of soil clay content and computed as

$$cfs2s3 = tcflow_{som2c(SOIL)} \times fps2s3 \times \left(1.0 + animpt \times \left(1.0 - anerb\right)\right) \qquad (2.151)$$

$$fps2s3 = ps2s3(1) + ps2s3(2) \times clay \qquad (2.152)$$

where *tcflow$_{som2c(SOIL)}$* is the total C flow out of *som2c(SOIL)* (g C m^{-2}, Eq. 2.148), *fps2s3* is the impact of clay on the flow (0 – 1), *animpt* is a slope term used to vary the impact of soil anaerobic conditions on decomposition flows to the passive soil organic matter pool (*fix.100* parameter), and *anerb* is the anaerobic effect (0 – 1, Eq. 2.28). The value of *fps2s3* increases with the *clay* fraction of mineral soil (0 – 1), and is modified by *fix.100* parameters, *ps2s3(1)* and *ps2s3(2)*. There is no microbial respiration associated with this flow since the flow into *som3c* is due to physical protection of organic matter by clay, and is not a biotic process (?).

The flow of *cfs2s3* from *som2c(SOIL)* to *som3c* is partitioned by isotope (csched). The amount of E flowing out of *som2e(SOIL,iel)* (*eflow$_{som2e(SOIL,iel)}$*, g E m^{-2}), and the amount of E flowing into *som3e(iel)* (*eflow$_b$*, g E m^{-2}) are calculated as

$$eflow_{som2e(SOIL,iel)} = cfs2s3 \times \frac{som2e(SOIL,iel)}{som2c(SOIL)} \qquad (2.153)$$

$$eflow_b = \frac{cfs2s3}{rcetob} \qquad (2.154)$$

$$mnrflow(iel) = eflow_{som2e(SOIL,iel)} - eflow_b \qquad (2.155)$$

where *rcetob* is the C/E ratio required by *som3c*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel)*.

Decomposition of *som2c(SOIL)* to *som1c(SOIL)*

The net C flow from *som2c(SOIL)* to *som1c(SOIL)* (*cfs2s1*, g C m^{-2}) is computed as

$$cfs2s1 = tcflow_{som2c(SOIL)} - co2los - cfs2s3 \qquad (2.156)$$

where $tcflow_{som2c(SOIL)}$ is the total C flow out of *som2c(SOIL)* (g C m^{-2}, Eq. 2.148), *co2los* is the respiration associated with the C flow from *som2c(SOIL)* (g C m^{-2}, Eq. 2.149), and *cfs2s3* is the net C flow from *som2c(SOIL)* to *som3c* (g C m^{-2}, Eq. 2.151)

The flow of *cfs2s1* from *som2c(SOIL)* to *som1c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *som2e(SOIL,iel)* ($eflow_{som1e(SOIL,iel)}$, g E m^{-2}), and the amount of E flowing into *som1e(SOIL, iel)* ($eflow_b$, g E m^{-2}) are calculated as

$$eflow_{som2e(SOIL,iel)} = cfs2s1 \times \frac{som2e(SOIL,iel)}{som2c(SOIL)} \tag{2.157}$$

$$eflow_b = \frac{cfs2s1}{rcetob} \tag{2.158}$$

$$mnrflow(iel) = eflow_{som2e(SOIL,iel)} - eflow_b \tag{2.159}$$

where *rcetob* is the C/E ratio required by *som1c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel) > 0*, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

2.9.4 Decomposition of *som2c(SRFC)* to *som1c(SRFC)* with CO$_2$ loss

If *aminrl(iel) > 10^{-7}* g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *som2c(SRFC)* is small enough to meet the required C/E of material flowing to *som1c(SRFC)* so that no immobilization occurs, then *som2c(SRFC)* can decompose.

The total C flow out of *som2c(SRFC)* ($tcflow_{som2c(SRFC)}$, g C m^{-2}) is calculated as

$$tcflow_{som2c(SRFC)} = som2c(SRFC) \times agdefac \times dec5(SRFC)$$
$$\times pHeff_{combination} \times mti \times dtm \tag{2.160}$$

where *agdefac* is the aboveground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), *dec5(SRFC)* is the intrinsic decomposition rate of *som2c(SRFC)* (yr^{-1}, *fix.100*), *pHeff$_{combination}$* is the pH effect on decomposition (0 – 1, Eq. 2.26), *mti* is the microbial turnover increase (1.0 – 5.0, Eq. 2.121), and *dtm* is the time step (fraction of a year, Eq. 2.2).

The respiration associated with the C flow from *som2c(SRFC)* (*co2los*, g C m^{-2}), and the mineralization of element *iel* (*mnrespflow(iel),* g E m^{-2}) associated with respiration, and net C flow from *som2c(SRFC)* to *som1c(SRFC)* (*cfs2s1*, g C m^{-2}) are calculated as

$$co2los = tcflow_{som2c(SRFC)} \times p2co2(SRFC) \tag{2.161}$$

$$mnrespflow(iel) = co2los \times \frac{som2e(SRFC,iel)}{som2c(SRFC)} \tag{2.162}$$

$$cfs2s1 = tcflow_{som2c(SRFC)} \times (1 - p2co2(SRFC)) \tag{2.163}$$

where $tcflow_{som2c(SRFC)}$ is the total C flow out of $som2c(SRFC)$ (g C m^{-2}, Eq. 2.160), and $p2co2(SRFC)$ is a $fix.100$ parameter $(0 - 1)$.

The flow of $cfs2s1$ from $som2c(SRFC)$ to $som1c(SRFC)$ is partitioned by isotope (csched). The amount of E flowing out of $som2e(SRFC,iel)$ ($eflow_{som1e(SRFC,iel)}$, g E m^{-2}), and the amount of E flowing into $som1e(SRFC, iel)$ ($eflow_b$, g E m^{-2}) are calculated as

$$eflow_{som2e(SRFC,iel)} = cfs2s1 \times \frac{som2e(SRFC,iel)}{som2c(SRFC)} \tag{2.164}$$

$$eflow_b = \frac{cfs2s1}{rcetob} \tag{2.165}$$

$$mnrflow(iel) = eflow_{som2e(SRFC,iel)} - eflow_b \tag{2.166}$$

where $rcetob$ is the C/E ratio required by $som1c(SRFC)$, calculated using the $agdrat$ function (Eq. 2.29), and $mnrflow(iel)$ (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If $mnrflow(iel) > 0$, net mineralization occurs and $mnrflow(iel)$ is added to $minerl(1,iel)$; otherwise, immobilization occurs and $mnrflow(iel)$ is removed from $minerl(1,iel)$.

2.9.5 Decomposition of *som3c* to *som1c(SOIL)* with CO$_2$ loss

The total C flow out of $som3c$ ($tcflow_{som3c}$, g C m^{-2}) is calculated as

$$tcflow_{som3c} = som3c \times bgdefac \times dec4 \times cltfac(3) \times anerb \\ \times pHeff_{fungi} \times dtm \tag{2.167}$$

where $bgdefac$ is the belowground decomposition factor based on water and temperature $(0 - 1$, Eq. 2.19), $dec4$ is the intrinsic decomposition rate of $som3c$ (yr^{-1}, $fix.100$), $cltfac(3)$ is the cultivation factor for $som3c$ (it equals $clteff(3)$ from $cult.100$ if cultivation has occurred in the past month, otherwise it equals 1.0), $anerb$ is the impact of soil

anaerobic conditions on decomposition (0 – 1, Eq. 2.28), $pHeff_{fungi}$ is the pH effect on decomposition (0 – 1, Eq. 2.26), and *dtm* is the time step (fraction of a year, Eq. 2.2).

If *aminrl(iel)* > 10^{-7} g E m^{-2} for each mineral (N, P, S) being simulated, or if the C/E ratio of *som3c* is small enough to meet the required C/E of material flowing to *som1c(SOIL)* so that no immobilization occurs, then *som3c* can decompose.

The respiration flux when *som3c* decomposes (*cf3co2*, g C m^{-2}), and the mineralization of element *iel* (*mnrespflow(iel)*, g E m^{-2}) associated with respiration, and net flow of C from *som3c* to *som1c(SOIL)* (*cfs3s1*, g C m^{-2}) are computed as

$$cf3co2 = tcflow_{som3c} \times p3co2 \tag{2.168}$$

(check code: I removed the *anerb* in the above equation because $tcflow_{som3c}$ calculation included *anerb*)

$$mnrespflow(iel) = cf3co2 \times \frac{som3e(iel)}{som3c} \tag{2.169}$$

$$cfs3s1 = tcflow_{som3c} \times (1.0 - p3co2) \tag{2.170}$$

where $tcflow_{som3c}$ is total C flow out of *som3c* (g C m^{-2}, Eq. 2.167), and *p3co2* is a *fix.100* parameter (0 – 1).

The flow of *cfs3s1* from *som3c* to *som1c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *som3e(iel)* ($eflow_{som3e(iel)}$, g E m^{-2}), and the amount of E flowing into *som1e(SOIL, iel)* ($eflow_b$, g E m^{-2}) are calculated as

$$eflow_{som3e(SOIL,iel)} = cfs3s1 \times \frac{som3e(SOIL,iel)}{som3c(SOIL)} \tag{2.171}$$

$$eflow_b = \frac{cfs3s1}{rcetob} \tag{2.172}$$

$$mnrflow(iel) = eflow_{som3e(iel)} - eflow_b \tag{2.173}$$

where *rcetob* is the C/E ratio required by *som1c(SOIL)*, calculated using the *bgdrat* function (Eq. 2.30), and *mnrflow(iel)* (g E m^{-2}) is the net mineralization or immobilization (**Figure FLOWS**). If *mnrflow(iel)* > 0, net mineralization occurs and *mnrflow(iel)* is added to *minerl(1,iel)*; otherwise, immobilization occurs and *mnrflow(iel)* is removed from *minerl(1,iel).*

2.9.6 Transfer of *som2c(SRFC)* into *som2c(SOIL)* due to mixing

The transfer of *som2c(SRFC)* to *som2c(SOIL)* due to mixing ($tcflow_{som2c(SRFC)}$, g C m^{-2}) is calculated as

$$tcflow_{som2c(SRFC)} = som2c(SRFC) \times mix \times agdefac \times dtm \tag{2.174}$$

where *mix* is the *cmix* parameter from *crop.100* for crop or savanna systems or the *tmix* parameter from *tree.100* for forest systems, *agdefac* is the aboveground decomposition factor based on water and temperature (0 – 1, Eq. 2.19), and *dtm* is the time step (fraction of a year, Eq. 2.2).

The flow of $tcflow_{som2c(SRFC)}$ from *som2c(SRFC)* to *som2c(SOIL)* is partitioned by isotope (csched). The amount of E flowing out of *som2e(SRFC,iel)* ($eflow_{som2e(SRFC,iel)}$, g E m^{-2}) and into *som2e(SOIL, iel)* ($eflow_b$, g E m^{-2}) is calculated as

$$eflow_{som2e(SRFC,iel)} = tcflow_{som2c(SRFC)} \times \frac{som2e(SRFC,iel)}{som2c(SRFC)} \tag{2.175}$$

where there is no mineralization or immobilization associated with this flow.

3 Trace Gas Submodel

3.1 Introduction

The bacterial processes of nitrification and denitrification are dominant sources of nitrous oxide (N_2O) and nitric oxide (NO). N_2O is a greenhouse gas with a 100-year time horizon global warming potential ~298 times that of CO_2 (Forster et al. 2007). NO is rapidly oxidized in air to nitrogen dioxide (NO_2), a major air pollutant. NO in the air may convert to nitric acid, which has been implicated in acid rain, and both NO and NO_2 participate in tropospheric ozone production. Furthermore, N_2O gives rise to NO.

Nitrification is the biological oxidation of ammonium (NH_4^+) to nitrite (NO_2^-) or nitrate (NO_3^-) under aerobic conditions. Under oxygen limited conditions nitrifying bacteria can use NO_2^- as a terminal e^- acceptor to avoid accumulation of the toxic NO_2^-, whereby N_2O and NO are produced. Denitrification is the reduction of NO_3^- or NO_2^- to gaseous N oxides and molecular N_2 by facultative heterotrophic bacteria. An important aspect of denitrification is the requirement for sufficient organic matter to drive the denitrification reaction. Since denitrifying bacteria are facultative organisms, they can use either dissolved O_2 or N oxides to serve as e^- acceptors during oxidation of labile C (e^- donor). The preferred nitrogen e^- acceptors in order of most to least thermodynamically favorable include NO_3^-, NO_2^-, NO, and N_2O. If dissolved O_2 and NO_3^- are present, bacteria will use the dissolved O_2 first. Therefore, denitrification occurs only under anaerobic or anoxic conditions. The nitrate reduction sequence under anaerobic conditions is described by Paul and Clark (1989):

$$NO_3^- \rightarrow NO_2^- \rightarrow NO^\uparrow \rightarrow N_2O^\uparrow \rightarrow N_2^\uparrow .$$
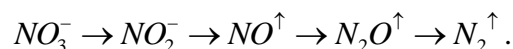
The trace gas model calculates the oxidation of NH_4^+, the reduction of NO_3^-, and the N_2O, NO, and N_2 gas fluxes associated with these two processes. The model simulates the pulse of NO due to the wetting of dry soils. It also incorporates a soil NO_3^- leaching (Figure 3.1). Additionally, it calculates methane (CH_4) oxidation in the soil. CH_4 is a greenhouse gas with a 100-year time horizon global warming potential ~21 times that of CO_2 (Forster et al. 2007). The trace gas model is called daily after decomposition calculations have been completed since the amount of N supplied by mineralization drives the nitrification and denitrification calculations.

Inputs to the nitrification calculations include soil ammonium concentration (μgN gsoil^{-1} or ppm N), volumetric soil water content (cm^3 H2O / cm^3 soil), water-filled pore space (WFPS, % relative saturation), minimum allowable volumetric soil water content (cm^3 H2O / cm^3 soil), volumetric field capacity (cm^3 H2O / cm^3 soil), soil temperature, soil pH, and soil bulk density (g cm^{-3}).

Inputs to the denitrification calculations include soil nitrate concentration (μgN gsoil^{-1} or ppm N), heterotrophic CO_2 respiration rate (μg C gsoil^{-1} day^{-1}), water-filled

pore space (WFPS, % relative saturation), soil temperature, soil bulk density (g cm^{-3}), soil texture, and volumetric field capacity (cm^3 H2O / cm^3 soil). The model assumes that denitrification rates are controlled by the availability of soil NO_3^-, labile C compounds (e^- donor), and O_2 (competing e^- acceptor). Heterotrophic respiration is used as a proxy for labile C availability. O_2 availability is a function of soil physical properties that influence gas diffusivity, soil WFPS, and O_2 demand. The potential O_2 demand, as indicated by respiration rates, to contribute to soil anoxia varies inversely with a soil gas diffusivity coefficient which is regulated by soil porosity and pore size distribution. The model selects the minimum of the NO_3^- and CO_2 functions to establish a maximum potential denitrification rate for particular levels of e^- acceptor and C substrate and accounts for limitation of O_2 availability to estimate daily $N_2 + N_2O$ flux rates. The ratio of soil NO_3^- concentration to CO_2 emissions was found to reliably model the ratio of N_2 to N_2O gases. The output of the ratio function is combined with the estimate of the total N gas flux rate to infer N_2O emissions (Del Grosso et al. 2000a).

The trace gas model has been documented in peer-reviewed journals and has used extensively in DayCent simulations cross the globe (Parton et al. 1996, Del Grosso et al. 2000a, Del Grosso et al. 2000b, Parton et al. 2001, Del Grosso et al. 2002, Del Grosso et al. 2005, Del Grosso et al. 2006, Del Grosso et al. 2008a, Del Grosso et al. 2008b, Del Grosso et al. 2009, Del Grosso et al. 2010).

3.2 Updating Soil Nitrate and Ammonium after Decomposition has Occurred

The first calculation of the trace gas model is to portion the new inorganic N from mineralization (*newminrl*, g N m^{-2}) into ammonium (*newNH$_4$*, g N m^{-2}) and nitrate (*newNO$_3$*, g N m^{-2}. (Note, the Century variable *minerl(lyr,N)* has already been updated in the decomposition subroutine, but *ammonium* (g N m^{-2}) and *nitrate$_{lyr}$* (g N m^{-2}) have not). If net immobilization occurs (*newminrl* ≤ 0), the loss of mineral N is distributed proportionally between ammonium and nitrate layers:

$$ammonium = ammonium + newminrl \times \frac{ammonium}{NpoolSum} \tag{3.1}$$

$$nitrate_{lyr} = nitrate_{lyr} + newminrl \frac{nitrate_{lyr}}{NpoolSum} \tag{3.2}$$

where *NpoolSum* is the sum of *ammonium* and *nitrate* in the soil (g N m^{-2}). The amount of *newminerl* that becomes ammonium and nitrate is calculated as

$$newNH_4 = \begin{cases} 0, & newminrl \leq 0 \\ newminrl \times (1.0 - netmn\_to\_no3), & newminrl > 0 \end{cases} \tag{3.3}$$

$$newNO_3 = \begin{cases} 0, & newminrl \leq 0 \\ newminrl \times (netmn\_to\_no3), & newminrl > 0 \end{cases} \tag{3.4}$$

where *netmn_to_no3* is the fraction of *newminrl* that is converted to nitrate (0 – 1). Note: *netmn_to_no3* currently set to 0.0, therefore all of *newminrl* becomes *newNH4*, and this is added to the *ammonium* pool (g N m^{-2}).

$$ammonium = ammonium + newNH_4 \tag{3.5}$$

3.3 Nitrification (nitrify.c)

3.3.1 Ammonium Concentration

Nitrification is the conversion of ammonium to nitrate with the release of N_2O and NO_x. The amount of *ammonium* (g N m^{-2}) that is nitrified (*nh4_to_no3*, g N m^{-2}) is a function of soil pH, soil moisture, and soil temperature. If the ammonium content of soil is less than *min_ammonium* (0.03 g N m^{-2}), then the amount of nitrification is zero and no further nitrification calculations are made.

$$nh4\_to\_no3 = 0 \qquad ammonium < min\_ammonium \tag{3.6}$$

To calculate *nh4_to_no3* (Eq. 3.17) when *ammonium* > *min_ammonium*, first convert *ammonium* (g N m^{-2}) to an ammonium concentration (*nh4_conc*, ppm N). This calculation assumes all ammonium occurs in the top 3 soil water layers (~top 15 cm of soil). The mass of soil under a 1-m^2 area from the soil surface to the bottom of the 3rd soil layer (*grams_soil*, g soil m^{-2}) is calculated from the bulk density of the layers (*bulkd$_{lyr}$*, g cm^{-3}) and the layer thickness (*width$_{lyr}$*, cm) as

$$grams\_soil = \sum_{lyr=0}^{2} bulkd_{lyr} \times width_{lyr} \times \left(100 \frac{cm}{m}\right)^2 \tag{3.7}$$

$$nh4\_conc = \frac{ammonium}{grams\_soil} \times \left(10^6 \frac{\mu g}{gram}\right) \tag{3.8}$$

3.3.2 The Effect of Soil Moisture on Nitrification

The effect of soil water on nitrification is based on relative water content when the soil is drier than field capacity and on water-filled pore space when the soil is wetter field capacity. The relative water content of a soil layer (*rel_wc$_{lyr}$*, 0 – 1.5) and water-filled porespace of a soil layer (*wfps$_{lyr}$*, 0 – 1) are calculated as

$$rel\_wc_{lyr} = \frac{\dfrac{swc_{lyr}}{width_{lyr}} - swclimit_{lyr}}{field_{lyr} - swclimit_{lyr}} \tag{3.9}$$

$$wfps_{lyr} = \frac{\dfrac{swc_{lyr}}{width_{lyr}}}{1.0 - \dfrac{bulkd_{lyr}}{PARTDENS}} \tag{3.10}$$

where swc_{lyr} is the soil water content of the layer (cm H_2O), $width_{lyr}$ is the thickness of the layer (cm), $fieldc_{lyr}$ is the volumetric soil water content of the layer at field capacity (0 – 1), $swclimit_{lyr}$ is the minimum volumetric soil water content of the layer (0 – 1), $bulkd_{lyr}$ is the bulk density of the layer (g m^{-3}), and *PARTDENS* is particle density (2.65 g cm^{-3}). The value of rel_wc_{lyr} is ≤ 1.0 when the soil water content of the layer is at field capacity or below and is > 1.0 when the soil water content of the layer is greater than field capacity; $wfps_{lyr}$ has a maximum value of 1.0 that occurs when the soil layer is saturated.

The effect of soil moisture on nitrification increases until soil water content approximately reaches field capacity (Figure 3.2a), then decreases linearly (Figure 3.2b). The effect of soil moisture on nitrification (*fNwfps*, 0 – 1) is calculated as

$$fNwfps = \begin{cases} \dfrac{1.0}{1.0 + 30.0 \times \exp(-9.0 \times avg\_rel\_wc)}, & avg\_rel\_wc \leq 1.0 \\[3mm] \dfrac{0.0 - 1.0}{(1.0 - avgfc)} \times (avgwfps - 1.0) + 0.0, & avg\_rel\_wc > 1.0 \end{cases} \tag{3.11}$$

where *avg_rel_wc* is the weighted average relative water content in the 2nd and 3rd soil water layers, *avgwfps* is the weighted average water-filled pore space in the 2nd and 3rd soil water layers (0 – 1), and *avgfc* is the weighted average volumetric soil water content at field capacity for the 2nd and 3rd soil water layers (0 – 1). The second value of *fNwfps* (above) is based on the line function with two known points (*x1,y1*) and (*x2,y2*) and another point (*x,y*) where *x* is known and *y* is unknown.

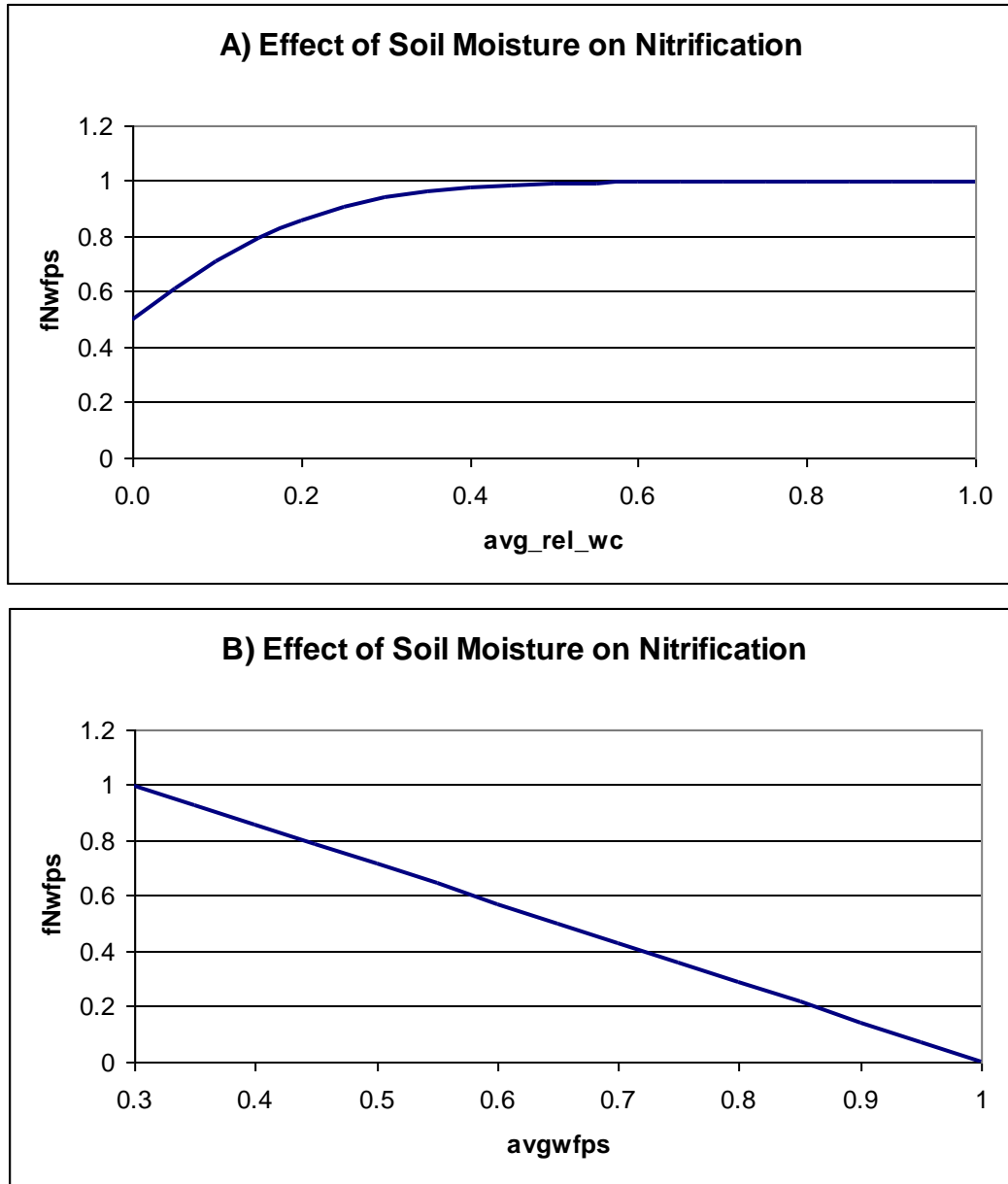$$y = \frac{y2 - y1}{x2 - x1} \times (x - x2) + y2. \tag{3.12}$$

Figure 3.2. A) The effect of average relative water content (*avg_rel_wc*) on nitrification, when *avg_rel_wc* ≤ 1. B) The effect of average water-filled pore space (*avgwfps*) on nitrification when *avg_rel_wc* > 1 assuming that average volumetric field capacity = 0.30. See Eq. 3.11.

3.3.3 The Effect of Soil Temperature on Nitrification

There are two functions used to calculate the effect of soil temperature on nitrification; the one selected depends on the long-term maximum monthly air temperature (*maxt*, ºC) (Figure 3.3). In both cases, the effect of soil temperature on

nitrification (*fNsoilt*, $0 - 1$) is a function of the average soil temperature of the 2nd and 3rd soil layers (*avgstemp*, ℃):

if *maxt* $\geq$ 35.0 then

$$fNsoilt = f\_gen\_poisson\_density\left(avgstemp, A_0, A_1, A_2, A_3\right)$$

(3.13)

$$= \left(\left(\frac{A_1 - avgsoiltemp}{A_1 - A_0}\right)^{A_2}\right) \times \exp\left(\frac{A_2}{A_3}\left(1.0 - \left(\frac{A_1 - avgsoiltemp}{A_1 - A_0}\right)^{A_3}\right)\right)$$

where $A_0 = maxt$, $A_1 = -5.0$, $A_2 = 4.5$, and $A_3 = 7.0$.

If *maxt* $<$ 35.0 then

$$fNsoilt = f\_gen\_poisson\_density\left(avgstemp + (A_0 - maxt), A_0, A_1, A_2, A_3\right)$$

(3.14)

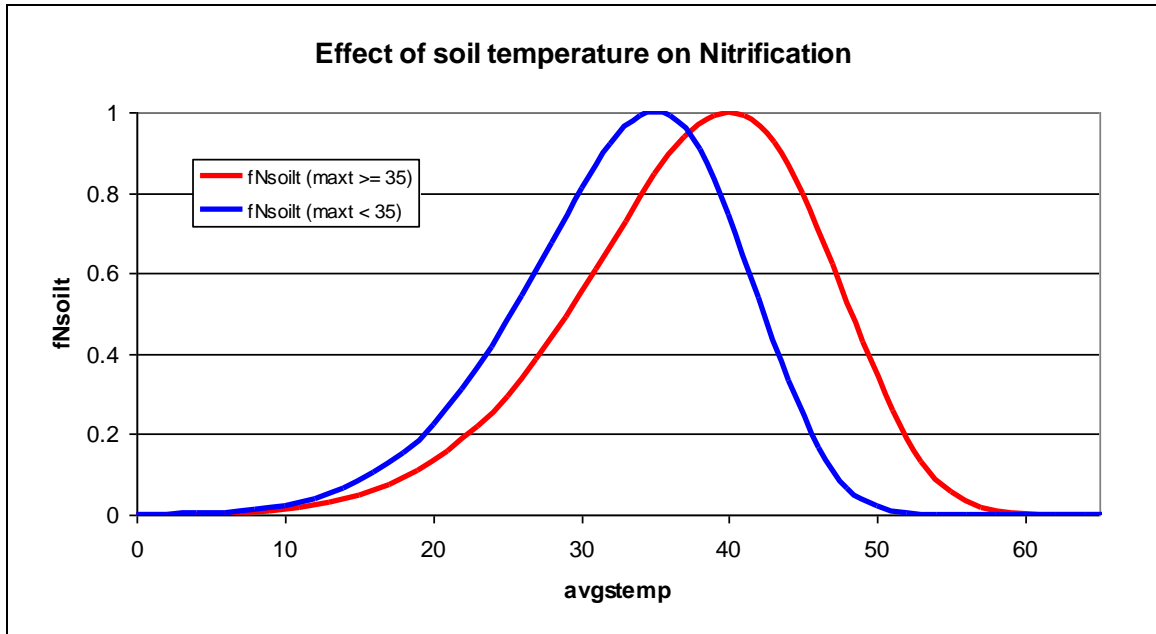where $A_0 = 35.0$, $A_1 = -5.0$, $A_2 = 4.5$, and $A_3 = 7.0$.

Figure 3.3. The effect of soil temperature on nitrification as a function of average soil temperature (*avgstemp*, ℃). The blue curves shows the function when the long-term maximum monthly air temperature (*maxt*) is $<$ 35 ℃ (in this case *maxt* = 30 ℃), and the red curve is the function when *maxt* $\geq$ 35 ℃ (in this case *maxt* = 40 ℃).

3.3.4 The Effect of Soil pH on Nitrification

Nitrification increases as soil pH becomes more basic. The effect of soil pH on nitrification (*fNph*, 0 – 1.4) is computed as

$$fNph = \begin{cases} 0, & pH < 5.0 \\ \text{f\_arctangent}\left(pH, A_0, A_1, A_2, A_3\right), & pH \geq 5.0 \\ A_1 + \dfrac{A_2}{\pi} \times \arctan\left(\pi \times A_3 \times \left(pH - A_0\right)\right) \end{cases} \qquad (3.15)$$

where *pH* is the soil pH in the second soil layer, $A_0 = 5.0$, $A_1 = 0.56$, $A_2 = 1.0$, and $A_3 = 0.45$ (Figure 3.4).
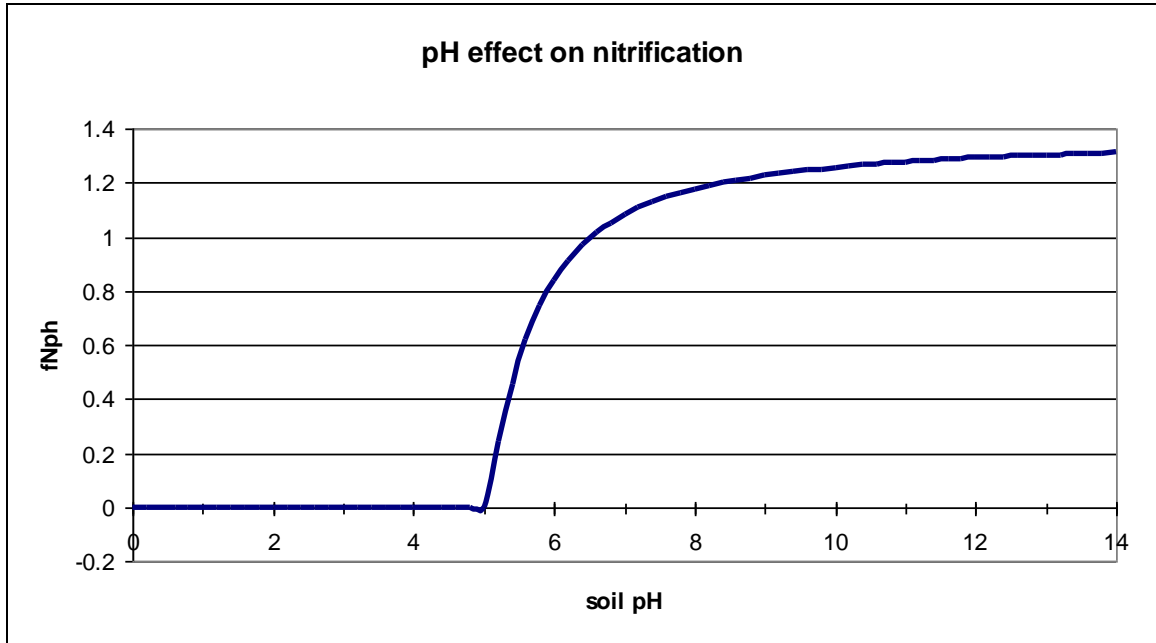

Figure 3.4. The effect of soil pH on nitrification. The function is set to zero for pH < 5.0.

3.3.5 The Effect of Ammonium Concentration on Nitrification

Nitrification is reduced as the ammonium concentration in the soil increases (?). The effect of the ammonium concentration on nitrification (*fNnh4*, 0 – 1) is computed as

$$fNnh4 \;=\; 1.0 \;-\; f\_exponential\left(nh4\_conc,\, A_0,\, A_1\right)$$
$$=\; 1.0 \;-\; A_0 \times \exp(A_1 \times nh4\_conc) \tag{3.16}$$

where $A_0 = 1.0$ and $A_1 = -0.0105$ (Figure 3.5).
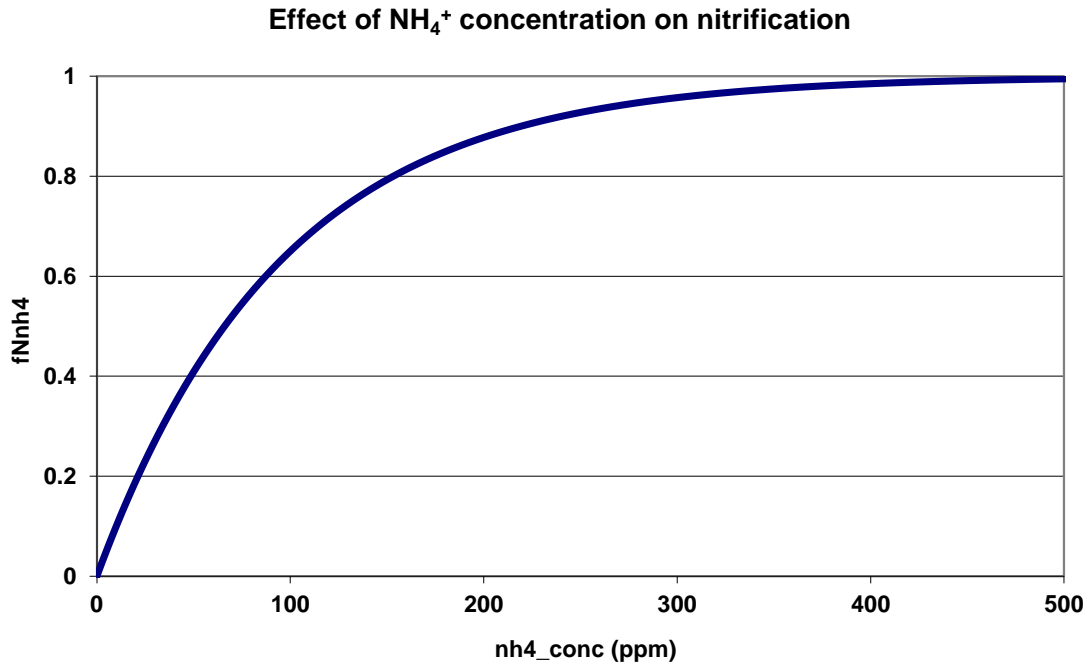.

Figure 3.5. The effect of ammonium concentration (*nh4_conc*, ppm N) on nitrification when $A_0 = 1.0$ and $A_1 = -0.0105$.

3.3.6 The Amount of Ammonium Converted to Nitrate by Nitrification

The amount of ammonium converted to nitrate by nitrification (*nh4_to_no3*, g N m^{-2} day^{-1}) is calculated as

$$nh4\_to\_no3 = absoluteMaxRate \times fNph$$
$$\times \max\left(fNwfps \times fNsoilt,\; Ncoeff\right) \times nreduce \tag{3.17}$$
$$+base\_flux$$

$$absoluteMaxRate = \min\left(0.4,\; ammonium \times MaxRate\right) \tag{3.18}$$

where *absoluteMaxRate* is the maximum amount of ammonium that can be nitrified in one day (g N m^{-2}), *MaxRate* is the maximum fraction of ammonium that goes to nitrate

during nitrification (0.15), *fNph* is the effect of soil pH on nitrification (0 − 1, Eq. 3.15), *fNwfps* is the soil moisture effect on nitrification (0 − 1, Eq. 3.11), *fNsoilt* is the soil temperature effect on nitrification (0 − 1, Eqs. 3.13 and 3.14), *Ncoeff* is the minimum water/temperature limitation coefficient for nitrification (0 − 0.1, sitepar.in), *nreduce* is the reduction factor on nitrification rates due to nitrification inhibitors added with fertilizer (0 − 1), and *base_flux* is equivalent to 0.1 g N ha^{-1} day^{-1} (0.1 x 10^{-4} g N m^{-2} day^{-1}).

The value of *nh4_to_no3* is reduced if it is greater than the difference between total soil ammonium and the minimum allowable soil ammonium content (*min_ammonium*, 0.03 g N m^{-2}), then is added to new nitrate (*newNO3*, g N m^{-2})

$$nh4\_to\_no3 = \min\left(nh4\_to\_no3,\ ammonium - min\_ammonium\right) \tag{3.19}$$

$$ammonium = ammonium - nh4\_to\_no3 \tag{3.20}$$

$$newNO3 = newNO3 + nh4\_to\_no3 \tag{3.21}$$

This completes calculations in subroutine nitrify.c.

3.3.7 N$_2$O and NO$_x$ from Nitrification

A fraction of the new nitrate from nitrification (*newNO3*, Eq. 3.21) will be converted to N$_2$O (*Nn2oflux*, g N m^{-2})

$$Nn2oflux = newNO3 \times turnovfrac \times N2Oadjust \tag{3.22}$$

$$newNO3 = newNO3 - Nn2oflux \tag{3.23}$$

where *turnovfrac* = 0.02, and *N2Oadjust* is the nitrification N$_2$O adjustment factor (0 − 1, *sitepar.in*).

The potential NOx flux from nitrification (*NOflux*, (g N m^{-2}) is proportional to *Nn2oflux* (g N m^{-2}, Eq. 3.22). The NO flux is determined by the NO to N$_2$O ratio (*NO_N2O_ratio*, g NO-N / g N$_2$O-N) (Figure 3.6) and is computed as

$$NO\_N2O\_ratio = \begin{cases} \dfrac{8.0 + 18.0 \times \arctan(0.75\pi(10.0 \times dDO - 1.86))}{\pi}, & isagri = false \\[4mm] 0.5 \times \dfrac{8.0 + 18.0 \times \arctan(0.75\pi(10.0 \times dDO - 1.86))}{\pi}, & isagri = true \end{cases}$$
$$\tag{3.24}$$

$$NOflux = NO\_N2O\_ratio \times Nn2oflux \times krainNO \tag{3.25}$$

where dDO is normalized diffusivity in aggregate soil media $(0 - 1)$ which is dependent on water-filled pore space (function diffuse.c,(Potter et al. 1996)); dDO increases as soil conditions become more aerobic. The boolean $isagri$ is true if the soil has ever been cultivated and is false otherwise, and $krainNO$ is the moisture and rain effect on the NOx flux $(0 - 4)$ (function nox_pulse.c, CITATION). The value if $krainNO$ is a minimum when there is snow cover and is a maximum when there is no snow cover and the soil receives a pulse of moisture after a dry period.
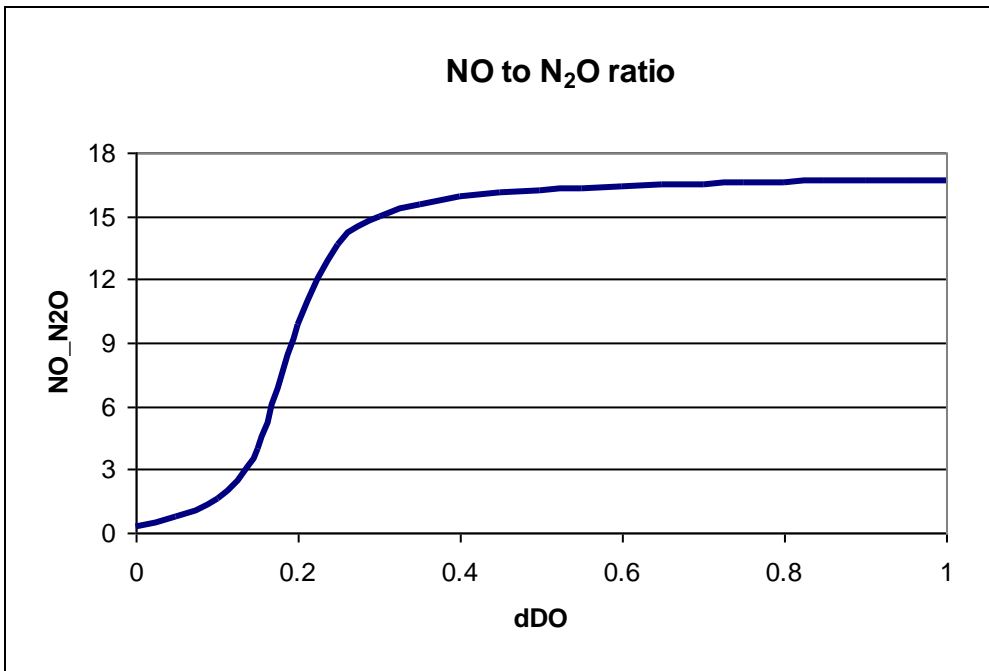

Figure 3.6. The NO to N₂O ratio as a function of soil diffusivity ($dD0$). The value if $dD0$ increases as soil conditions become more aerobic.

As with the N₂O flux from nitrification($Nn2oflux$, Eq. 3.23), the source of N for $NOflux$ from nitrification (Eq. 3.25) comes from $newNO3$,

$$newNO3 = newNO3 - NOflux. \tag{3.26}$$

If there is not enough N in $newNO3$ to balance the $NOflux$, N is removed from the $ammonium$ pool as well; $NOflux$ is reduced if the $ammonium$ pool is also too small to provide N for the flux. Any of the $newNO3$ remaining after N is removed for N₂O and NOₓ fluxes is added to soil nitrate; $newNO3$ is distributed to all soil nitrate layers based on the proportion of roots in each layer. After $newNO3$ is distributed to the soil, the leaching of nitrate between soil layers is calculated as described in the following section.

3.4 Nitrate Leaching (leachdly.c)

The amount of nitrate leaching ($amtlea_{lyr}$, g N m^{-2}) from a soil layer (lyr) to the one below it ($lyr + 1$) occurs when the flow of water out of the bottom of lyr ($wfluxout_{lyr}$, cm H$_2$O day^{-1}) is positive and soil nitrate in the layer $nitrate_{lyr}$, g N m^{-2}) is positive. (Note: The values of $wfluxout_{lyr}$ are computed by the soilwater model; $wfluxout_{lyr} < 0$ indicates an upward flux of water from evaporation). If $wfluxout_{lyr} \leq 0$ or $nitrate_{lyr} \leq 0$

$$amtlea_{lyr} = 0.$$

If $wfluxout_{lyr} > 0$ and $nitrate_{lyr} > 0$, $amtlea_{lyr}$, is calculated from the leaching intensity ($linten$, $0 - 1$)

$$linten = \min\left(1.0 - \frac{critflow - wfluxout_{lyr}}{critflow}, \ 1.0\right)$$

(3.27)

$$linten = \max(linten, \ 0.0)$$

$$amtlea_{lyr} = frlechd_N \times nitrate_{lyr} \times linten \tag{3.28}$$

where $critflow$ is the minimum amount water flow for leaching of minerals (it is equal to $minlch$, $fix.100$, cm H$_2$O day^{-1}) and $frlechd_N$ is the leaching fraction for N ($0 - 1$). The value $frlechd_N$ increases with the soil $sand$ fraction ($0 - 1$) and is computed in subroutine dailymoist as

$$texeff = fleach(1) + fleach(2) \times sand \tag{3.29}$$

$$frlechd_N = texeff \times fleach(3) \tag{3.30}$$

where $texeff$ is the texture effect ($0 - 1$) and $fleach(*)$ are $fix.100$ parameters.

For the bottom soil layer ($numlyrs - 1$), the amount of N that leaches into stream flow ($strmN$, g N m^{-2} day^{-1}) is computed as

$$strmN = \begin{cases} 0, & lyr < numlyrs - 1 \\ amtlea_{lyr} \times stormf, & lyr = numlyrs - 1 \end{cases} \tag{3.31}$$

where $stormf$ is the fraction of N leached into stormflow ($<site>.100$).

The amount of N leached is transferred to from the nitrate pool in *lyr* to the nitrate pool in *lyr+1*.

$$nitrate_{yr} = nitrate_{lyr} - amtlea_{lyr}$$

(3.32)

$$nitrate_{lyr+1} = \begin{cases} nitrate_{lyr+1} + amtlea_{lyr}, & lyr < numlyrs - 1 \\ nitrate_{lyr+1} + \left(amtlea_{lyr} - strmN \right), & lyr = numlyrs - 1 \end{cases}$$

The base flow N (*baseN*, g N m^{-2} day^{-1}) is computed when the pool of nitrate below the soil profile is positive

$$baseN = \begin{cases} 0, & lyr < numlyrs \\ nitrate_{lyr} \times basef, & lyr = numlyrs \end{cases}$$

(3.33)

$$nitrate_{lyr} = nitrate_{lyr} - baseN$$

(3.34)

where *basef* is the fraction of N leached into baseflow (0 – 1, *<site>.100*). The total amount of inorganic N leached into the stream (*inorglch*, g N m^{-2} day^{-1}) is calculated as

$$inorglch = strmN + baseN .$$

(3.35)

3.5 Denitrification (denitrify.c)

Denitrification occurs in anaerobic environments and reduces soil nitrate, producing N$_2$O and N$_2$ gases. Total N loss during denitrification is controlled by soil water content, available soil carbon, and soil nitrate (NO$_3^-$). The fraction of total N loss that is N$_2$ or N$_2$O is controlled by these same three factors. Unlike nitrification that was calculated for the top 15 cm of soil as a whole, denitrification is calculated for each DayCent soil layer in the soil profile, and the contribution from each soil layer is summed to compute total N$_2$O flux.

3.5.1 The Soil Nitrate Concentration

The soil nitrate content of each soil water layer (*nitrate_{lyr}*, g N m^{-2}) is converted to soil nitrate concentrations (*nitratePPM*, ppm N). The mass of soil under a 1-m^2 area in any soil layer (*grams_soil_{lyr}*, g soil m^{-2}) is calculated from the bulk density of the layer (*bulkd_{lyr}*, g cm^{-3}) and the layer thickness (*width_{lyr}*, cm).

$$nitratePPM_{lyr} = \frac{nitrate_{lyr}}{grams\_soil_{lyr}} \times \left(10^6 \frac{\mu g}{gram} \right) \tag{3.36}$$

$$grams\_soil_{lyr} = bulkd_{lyr} \times width_{lyr} \times \left(100 \frac{cm}{m} \right)^2 \tag{3.37}$$

If $nitratePPM_{lyr}$ (ppm N) is less than the minimum nitrate concentration required in a soil layer for denitrification ($min\_nitrate$, 0.1 ppm N), then the denitrification the sum of N gas fluxes ($N_2 + N_2O$) for the current layer ($Dtotflux_{lyr}$, ppm N) is equal to zero and the remaining calculations for the soil layer are skipped.

$$Dtotflux_{lyr} = 0 \qquad nitratePPM_{lyr} < min\_nitrate \tag{3.38}$$

3.5.2 The Effect of Soil CO$_2$ Concentration on Denitrification

The heterotrophic respiration rate is used as a proxy for labile C availability. The concentration of CO$_2$ in a soil layer ($co2PPM_{lyr}$, ppm) is calculated as

$$co2PPM_{lyr} = \frac{k_{lyr} \times newCO2}{grams\_soil_{lyr}} \times \left(10^6 \frac{\mu g}{gram} \right) \tag{3.39}$$

where k_{lyr} is the proportion of $newNO3$ to distribute to soil each layer (it is equal to the fraction of roots for the layer, Table 1.1), $newCO2$ is the amount of microbial soil respiration that has occurred in the past day (g C m^{-2} day^{-1}), and $grams\_soil_{lyr}$ (g soil m^{-2}) is the grams of soil in the layer under a 1-m^2 area. When water-filled pore space has reached a threshold value ($WFPS\_threshold$), a corrected CO$_2$ concentration for the soil layer ($co2\_correction_{lyr}$) is calculated as

$$WFPS\_threshold = \begin{cases} 0.80 & dD0\_fc_{lyr} \geq 0.15 \\ \dfrac{dD0\_fc_{lyr} \times 250 + 43}{100} & dD0\_fc_{lyr} < 0.15 \end{cases} \tag{3.40}$$

$$dD0\_fc_{lyr} = diffusiv\left(fieldc_{lyr}, \ bulkd_{lyr}, \ wfps\_fc_{lyr} \right) \tag{3.41}$$

$$co2\_correction_{lyr} = \begin{cases} co2PPM_{lyr} & wfps_{lyr} \leq WFPS\_threshold \\ co2PPM_{lyr}\left(1.0 + 100a\left(wfps_{lyr} - WFPS\_threshold\right)\right) & wfps_{lyr} > WFPS\_threshold \end{cases}$$
$$\tag{3.42}$$

$$a = \begin{cases} 0.004 & dD0\_fc_{lyr} \geq 0.15 \\ -0.1 \times dD0\_fc_{lyr} + 0.019 & dD0\_fc_{lyr} < 0.15 \end{cases}$$ (3.43)

where $dD0\_fc_{yr}$ is the soil gas diffusivity at field capacity $(0-1)$ of the soil layer (Eq. 3.41, (Potter et al. 1996)) and $wfps_{lyr}$ is the actual water-filled pore space of the soil layer $(0-1)$. The value of $dD0\_fc_{yr}$ is computed the properties of the soil layer including field capacity ($fieldc_{lyr}$, $0-1$), the bulk density ($bulkd_{lyr}$), and the water-filled pore space at field capacity ($wfps\_fc_{lyr}$, $0-1$).

3.5.3 The Effect of Soil Nitrate on Denitrification

Denitrification increases with soil nitrate concentration. The effect of soil nitrate on denitrification for the soil layer ($fDno3_{lyr}$, ppm N day^{-1}) is computed as

$$\begin{aligned} fDno3_{lyr} &= \text{f\_arctangent}\left(nitratePPM_{lyr},\ A_0,\ A_1,\ A_2,\ A_3\right) \\ &= A_1 + \frac{A_2}{\pi} \times \arctan\left(\pi \times A_3 \times \left(nitratePPM_{lyr} - A_0\right)\right) \end{aligned}$$ (3.44)

where $nitratePPM_{lyr}$ is the soil nitrate concentration in the soil layer (ppm N, Eq. 3.36), $A_0 = 9.23$, $A_1 = 1.556$, $A_2 = 76.91$, and $A_3 = 0.00222$ (Figure 3.7) (Del Grosso et al. 2000a).
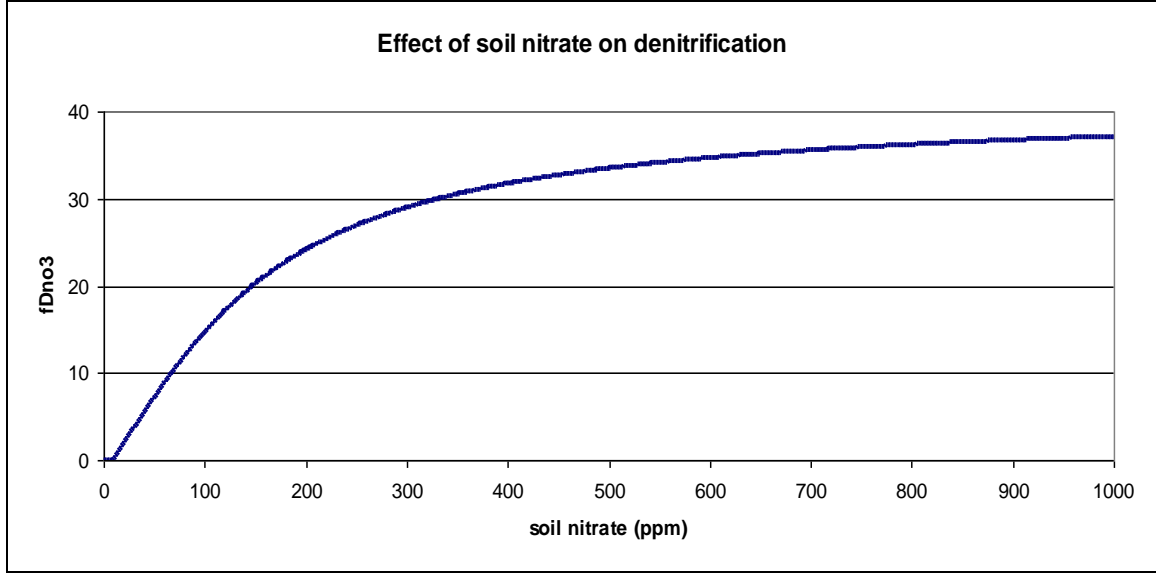
Figure 3.7. The effect of soil nitrate concentration on denitrification.

3.5.5 The CO_2 Effect on Denitrification

The CO_2 effect on denitrification ($fDco2_{lyr}$, ppm N day^{-1}) takes into account the corrected CO_2 concentration (Eq. 3.42) (citation?):

$$fDco2_{lyr} = \max\left(0.0, \left(0.1 \times \left(co2\_correction_{lyr}\right)^{1.3} - min\_nitrate\right)\right) \tag{3.45}$$

where *min_nitrate* is the minimum nitrate concentration required in a soil layer for denitrification (0.1 ppm N).

3.5.6 The Soil Moisture Effect on Denitrification

The soil moisture effect on denitrification for the soil layer ($fDwfps_{lyr}$, $0 - 1$) is computed from $wfps_{lyr}$ (Del Grosso et al. 2000a) (**Figure 3.8**):

$$fDwfps_{lyr} = 0.45 + \frac{\arctan\left(0.6\pi\left(10.0 \times wfps_{lyr} - x\_inflection_{lyr}\right)\right)}{\pi} \tag{3.46}$$

$$M = \min\left(0.113, \ dD0\_fc\right) \times \left(-1.25\right) + 0.145 \tag{3.47}$$

$$x\_inflection_{lyr} = 9.0 - M \times co2\_correction_{lyr} \tag{3.48}$$

where the *x_inflection* calculation for the soil layer uses the a multiplier function (*M*) and corrected CO_2 concentration (*co2_correction$_{lyr}$*, Eq. 3.42). (Note: Eqs. 3.46 – 3.48 have been modified slightly since Del Grosso et al. (2000a) –see Figure 7a, Figure 6a, and Eq. 3 in that paper).
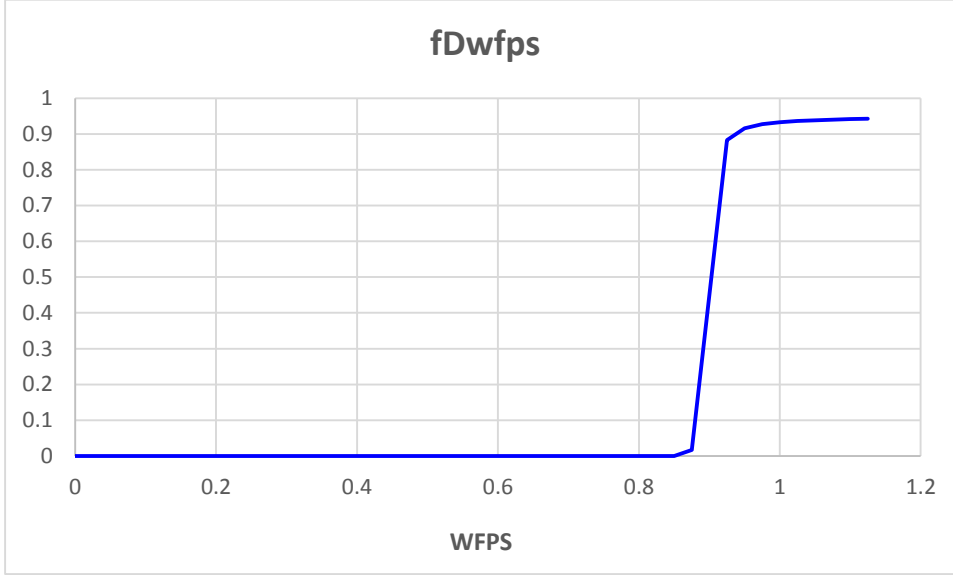

Figure 3.8. Example of the water-filled pore space effect on denitrification. In this example, *dDO_fc* = 0.113 and *co2_correction* = 0.0077.

The total N gas loss (N_2 + N_2O) for the current layer *(Dtotflux$_{lyr}$*, ppm N) assumes that denitrification is controlled by the molecular species (NO_3^- or labile C) that is most limiting. *Dtotflux$_{lyr}$* is computed from the effects of soil nitrate (*fDno3$_{lyr}$*, ppm N day^{-1}, Eq. 3.44), soil CO_2 (*fDco2$_{lyr}$* , ppm N day^{-1}, Eq. 3.45), and soil moisture (*fDwfps$_{lyr}$*, 0 – 1, Eq. 3.46):

$$fDno3\_co2_{lyr} = \begin{cases} fDno3_{lyr} & jdayStart \leq jday \leq jdayEnd \\ \min\left(fDno3_{lyr}, fDco2_{lyr}\right) & otherwise \end{cases} \quad (3.49)$$

$$Dtotflux_{lyr} = \begin{cases} fDwfps_{lyr} \times \max(0.066, fDno3\_co2_{lyr}) & lyr = 0,1 \\ fDwfps_{lyr} \times fDno3\_co2_{lyr} & lyr \geq 2 \end{cases} \quad (3.50)$$

where *fDno3_co2$_{lyr}$* is the limiting effect of soil NO_3^- and soil CO_2; it does not include CO_2 effect on denitrification between given Julian days *jdayStart* and *jdayEnd* (*sitpar.in*) if these two parameters have been specified (WHY?). The minimum value for potential denitrification in top 2 soil layers is 0.066 ppm N.

3.5.7 The N_2/N_2O Ratio

Nitrate and CO_2 effect on the N_2/N_2O Ratio

The nitrate and CO_2 effect on the ratio of N_2 to N_2O (*fRno3_co2*) is a function of the ratio of e^- acceptor (NO_3^-) to CO_2 emission (a proxy for e^- donor availability) (Del Grosso et al. 2000a):

$$k1 = \max\left(1.5,\ 38.4 - 350 \times dD0\_fc\right) \tag{3.51}$$

$$fRno3\_co2 = \max\left(0.16 \times k1,\ k1 \times \exp\left(\frac{-0.8 \times nitratePPM_{lyr}}{co2PPM_{lyr}}\right)\right) \tag{3.52}$$

where *k1* is a parameter controlling the maximum value of *fRno3_co2* and *dD0_fc* is soil gas diffusivity at field capacity (Eq. 3.41). The intercept of *fRno3_co2* is a function of *dD0_fc* in intact soils (see Figure 7c in Del Grosso et al. (2000a)). (Note: Eq. 3.51 has been modified slightly since Del Grosso et al. (2000a) – see *k1* calculation in Figure 6b in that paper).

Water-Filled Pore Space effect on the N_2/N_2O Ratio

The water-filled pore space effect on the N_2/N_2O ratio (*fRwfps*, Figure 5h in Del Grosso et al. (2000a)) is a function of *wfps$_{lyr}$*:

$$fRwfps = \max\left(0.1,\ 0.015 \times 100 \times wfps_{lyr} - 0.32\right). \tag{3.53}$$

N_2/N_2O Ratio calculation

The N_2/N_2O Ratio for the soil layer (*Rn2n2o$_{lyr}$*, Eq. 4 in Del Grosso et al. (2000a)) has a minimum value of 0.1 and is computed as:

$$Rn2n2o_{lyr} = \max\left(0.1,\ fRno3\_co2_{lyr} \times fRwfps_{yr}\right) \tag{3.54}$$

where *fRno3_co2$_{lyr}$* is the soil NO_3^-/CO_2 effect (Eq. 3.52) and *fRwfps* is the soil moisture effect (Eq. 3.53).

3.5.8 N_2 and N_2O Fluxes from Denitrification

Denitrification N_2 (*dN2Olyr,* gN m^{-2}) and denitrification N_2O flux (*dN2Olyr,* gN m^{-2}, see Eq. 5 in Del Grosso et al. (2000a)) for the soil layer are computed from the total N flux *(Dtotflux$_{lyr}$*, ppm N, Eq. 3.50) and the N_2/N_2O Ratio (*Rn2n2o$_{lyr}$*, Eq. 3.54), converting ppm N to g N m^{-2}.

$$dN2O_{lyr} = \left(Dtotflux_{lyr} \times grams\_soil_{lyr} \times 10^{-6} \frac{gram}{\mu g} \right) \left(\frac{1}{Rn2n2o + 1.0} \right)$$

(3.55)

$$dN2_{lyr} = \left(Dtotflux_{lyr} \times grams\_soil_{lyr} \times 10^{-6} \frac{gram}{\mu g} \right) \left(1 - \frac{1}{Rn2n2o + 1.0} \right)$$

The nitrate in soil layer is reduced by the amount of N_2-N and N_2O-N ($dN2O_{lyr} + dN2_{lyr}$). The nitrate concentration of any layer is not permitted to fall below *min_nitrate_end* (0.05 ppm N); $dN2O_{lyr}$ and $dN2_{lyr}$ are reduced if necessary.

The total N_2 and N_2O fluxes for the day (*Dn2flux* and *Dn2oflux*, g N m^{-2} day^{-1}) are the sum of fluxes from each soil layer.

$$Dn2\,flux = \sum_{lyr} dN2_{lyr}$$

(3.56)

$$Dn2oflux = \sum_{lyr} dNO2_{lyr}$$

This concludes the calculations in denitrify.c.

3.5.9 NOx flux from Denitrification

The maximum possible NO flux (*potentialNOflux*, g N m^{-2} day^{-1}) is based on the NO/N_2O ratio (Eq. 3.24) (**Figure 3.9**) and the moisture and rain pulse effect on the NOx flux (*krainNO*, 0 – 4) (function nox_pulse.c, CITATION), and is proportional to *Dn2oflux* (g N m^{-2} day^{-1}).

$$NOtoN_2Oratio = 8.0 + \frac{18.0 * atan(0.75 * \pi * (10 * dDO - 1.86))}{\pi}$$

(3.57a)

$$potentialNOflux = NOtoN2Oratio \times Dn2oflux \times \min(1.0,\ krainNO)$$

(3.57)

Actual NO flux will be $\leq$ *potentialNOflux*, depending on the amount of ammonium in the soil. If *potentialNOflux* $\leq$ *ammonium*, then *potentialNOflux* is added to total NO flux (*NOflux*, g N m^{-2} day^{-1}, Eq. 3.25), and the N for the flux is taken from the ammonium pool:

$$NOflux = NOflux + potentialNOflux$$

(3.58)

$$ammonium = ammonium - potentialNOflux$$

If *potentialNOflux > ammonium,* remove the rest of the available *ammonium,* then convert some *Dn2oflux* to *NOflux*

$$NOflux = NOflux + ammonium$$
$$potentialNOflux \ = \ potentialNOflux - ammonium$$ (3.59)
$$ammonium = 0$$

if $potentialNOflux \ \le Dn2oflux$

$$NOflux = NOflux + potentialNOflux$$
(3.60)
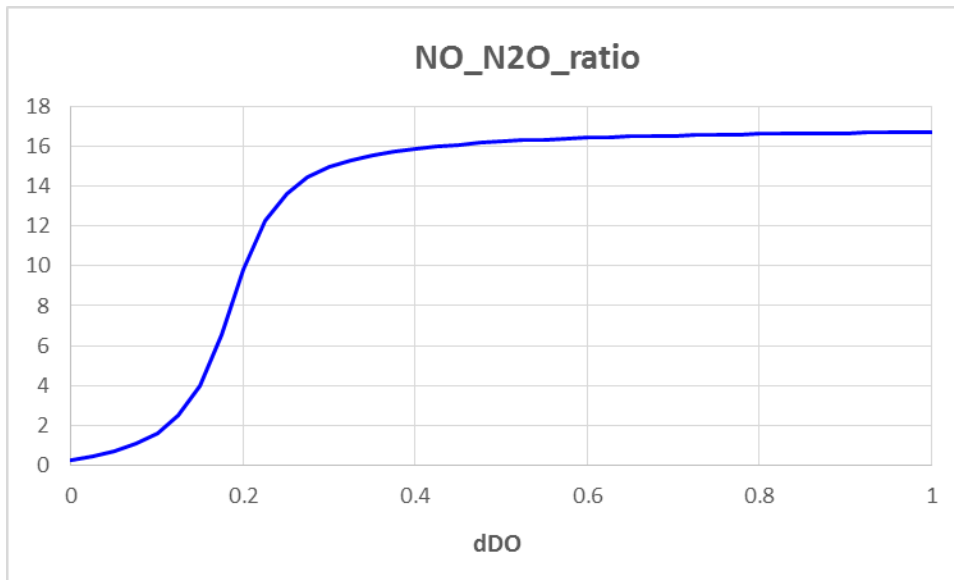$$Dn2oflux = Dn2oflux - potentialNOflux$$

Figure 3.9. The NOx to N$_2$O ratio (eq. 3.57a) based on diffusivity (*dDO*). For agriculture this ratio is halved.

3.5.10 NO$_x$ flux Absorbed by the Vegetation Canopy

The amount of the NO flux that is absorbed by leaves of plants in computed from the sum of LAI of grasses (*grassLAI*) and trees (*treeLAI*)

$$totalLAI = grassLAI + treeLAI \tag{3.61}$$

If $totalLAI > 0.0$, the amount of NO absorbed by leaves ($NOabsorp$, gN m^{-2}) is calculated as

$$canopyReduction = 0.0077 \times totalLAI^2 - 0.13 \times totalLAI + 0.99 \tag{3.62}$$

$$NOabsorp = \begin{cases} 0, & totLAI = 0 \\ NOflux \times (1 - canopyReduction), & totLAI > 0 \end{cases} \tag{3.63}$$

$$NOabsorpGrass = NOabsorp \times \frac{grassLAI}{totalLAI} \tag{3.64}$$

$$NOabsorpTree = NOabsorp \times \frac{treeLAI}{totalLAI} \tag{3.65}$$

where *NOflux* is the total NO flux from nitrification and denitrification (g N m^{-2} day^{-1}, Eqs. 3.25, and 3.58 or 3.59).

3.6 Methane Oxidation

Methane oxidation is a function of soil temperature, soil water content, porosity, and field capacity. The methane oxidation model of DayCent (Del Grosso et al. 2000b) is based on soil characteristics in the top 15 cm (CH$_4$DEPTH) of soil profile including fixed soil properties such as field capacity (*fieldcapacity*) and bulk density (*bulkdensity*), and transient soil properties including daily mean soil temperature (*soiltemp*), water-filled pore space (*wfps*), and volumetric soil water content (*soilwater)*. The soil diffusivity function used by the model (*diffusiv*) computes the estimated normalized diffusivity in soils as a function of soil porosity and field capacity and is based on the method of Potter et al. (1996). There two separate sets of calculations: one for deciduous forests and one for grasslands, tropical forests, coniferous forests, and agricultural lands

3.6.1 CH$_4$ Oxidation for a Deciduous Forest

$CH_4\,max$ is the maximum CH$_4$ oxidation rate (g C ha^{-1} day^{-1}). The actual CH$_4$ oxidation rate will be reduced by a soil temperature effect and a soil moisture effect. For a deciduous forest, CH_4max is calculated as

$$CH_4max = 40.0 - 18.3 \times bulkdensity \tag{3.66}$$

where *bulkdensity* is the average bulk density of the top CH4DEPTH cm of soil (g cm^{-3}). See Figure 7a from Del Grosso et al. (2000b), below.

The soil temperature effect on CH$_4$ oxidation for a deciduous forest (*tempAdjust*, $0 - 1$) is computed as

$$tempAdjust = 0.0209 \times soiltemp + 0.845 \quad\quad\quad (3.67)$$

where *soiltemp* is the average soil temperature in the top CH4DEPTH cm of soil (ºC). See Figure 7c from Del Grosso et al. (2000b), below.

The soil moisture effect for a deciduous forest (*wfpsAdjust*, $0 - 1$) is bounded when the average water-filled pore space in the top CH4DEPTH cm of soil (*wfps*, $0 - 1$) falls below a critical value:

If *wfps* ≤ 0.05 then

$$wfpsAdjust = 0.1$$

If *wfps* > 0.05 then

$$wfpsAdjust = \left(\frac{10 \times wfps - 0.5}{1.84 - 0.5}\right)^{0.13} \times \left(\frac{10 \times wfps - 55}{1.84 - 55}\right)^{0.13 \times \frac{55 - 1.84}{1.84 - 0.5}} \quad\quad (3.68)$$
$$= \max\left(0.1, \ wfpsAdjust\right)$$

See Figure 7b from Del Grosso et al. (2000b), below.

The actual CH$_4$ oxidation rate for a deciduous forest (*CH4flux*, g C ha^{-1} day^{-1}) is a product of the maximum CH$_4$ oxidation rate (*CH4max*, g C ha^{-1} day^{-1}, Eq. 3.66), the water adjustment factor (*wfspAdjust*, Eq. 3.68), and the temperature adjustment factor (*tempAdjust*, Eq. 3.67):

$$CH_4flux = CH_4max \times wfpsAdjust \times tempAdjust. \quad\quad\quad (3.69)$$

See Eq. 3 in Del Grosso et al. (2000b).

3.6.2 CH$_4$ Oxidation for Grasslands, Coniferous Forests, Tropical Forests, or Agricultural Systems

For grasslands, coniferous forests, tropical forests, or agricultural systems, the maximum volumetric soil water content for CH$_4$ oxidation (*Wmax*, $0 - 50\%$), the minimum volumetric soil water content for CH$_4$ oxidation (*Wmin*, $0 - 50\%$), and the optimum volumetric soil water content for CH$_4$ oxidation (*Wopt*, $0 - 50\%$, See Figure 2a

in Del Grosso et al. (2000b), below) are functions of volumetric field capacity (*fieldcapacity*, $0-1$):

$$Wmin = 3.0 \times fieldcapacity - 0.28$$
$$Wopt = 6.3 \times fieldcapacity - 0.58 \tag{3.70}$$
$$Wmax = 10.6 \times fieldcapacity + 1.9$$

See also Figure 5a from Del Grosso et al. (2000b), below.

The maximum rate for CH$_4$ oxidation rate for grasslands, coniferous forests, tropical forests, or agricultural systems (*CH$_4$max*, g C ha^{-1} day^{-1}) is calculated as

$$CH_4max = 53.8 \times Dopt + 0.58 . \tag{3.71}$$

$$Dopt = diffusiv \left(fieldcapacity, \ bulkdensity, \ \frac{0.1 \times Wopt}{1.0 - \dfrac{bulkdenisty}{PARTDENSITY}} \right) \tag{3.72}$$

where *Dopt* $(0-1)$ is the soil gas diffusivity through soil assuming an optimum water content (*Wopt*). See Figure 2b from Del Grosso et al. (2000b), below.

The effect of soil moisture for grasslands, coniferous forests, tropical forests, or agricultural systems (*watrAdjust*, $0-1$) attenuates the maximum rate of CH$_4$ oxidation. If $Wmin \le 0.1*soilwater \le Wmax$ then

$$watrAdjust = \left(0.1 \times \frac{soilwater - Wmin}{Wopt - Wmin} \right)^{0.4} \times \left(0.1 \times \frac{soilwater - Wmax}{Wopt - Wmax} \right)^{0.4 \times \frac{Wmax - Wopt}{Wopt - Wmin}} \tag{3.73}$$
$$= \max \left(0.1, \ watrAdjust \right)$$

otherwise, when $0.1*soilwater < Wmin$ or $0.1*soilwater > Wmax$ then

$$watrAdjust = 0.1 .$$

where *soilwater* is the average soil water content in the top CH$_4$DEPTH cm of soil ($0-50\%$). See Figure 5a from Del Grosso et al. (2000b), below.

Agricultural areas have reduced methane consumption since plowing and fertilization tend to depress CH$_4$ oxidation. If the system is agricultural, the agricultural adjustment factor (*agriAdjust*, $0.0-1.0$) will be < 1.0, and the value is further refined by the value of *Dopt:*

$$agriAdjust = \begin{cases} 0.90 & Dopt < 0.15 \\ -4.6 \times Dopt + 1.6 & 0.15 \le Dopt \le 0.28 \\ 0.28 & Dopt > 0.28 \end{cases} \qquad (3.74)$$

where *Dopt* is the soil gas diffusivity through soil assuming an optimum water content (*Wopt*, 0 − 1, Eq. 3.72). If the system is not agricultural, then *agriAdjust* = 1.0. See Figure 5c from Del Grosso et al. (2000b), below.

The effect of soil temperature for grasslands, coniferous forests, tropical forests, or agricultural systems (*tempAdjust*, 0 − 1) also attenuates the maximum rate of CH_4 oxidation:

$$tempAdjust = \left(soiltemp \times \max\left(0.11,\ Dopt\right) \times 0.095 \right) + 0.9 \qquad (3.75)$$

where *soiltemp* is the average soil temperature in the top CH_4DEPTH cm of soil (ºC). See Figure 5b from Del Grosso et al. (2000b), below.

The actual CH_4 oxidation rate (*CH₄flux*, g C ha^{-1} day^{-1}) for grasslands, coniferous forests, tropical forests, agricultural systems is a product of the maximum CH_4 oxidation rate (*CH₄max*, g C ha^{-1} day^{-1}, Eq. 3.71) and the water, temperature, and agricultural adjustment factors (Eqs. 3.73, 3.75, and 3.74, respectively):

$$CH_4\,flux = CH_4max \times watrAdjust \times tempAdjust \times agriAdjust. \qquad (3.76)$$

See Eq. 2 in Del Grosso et al. (2000b).

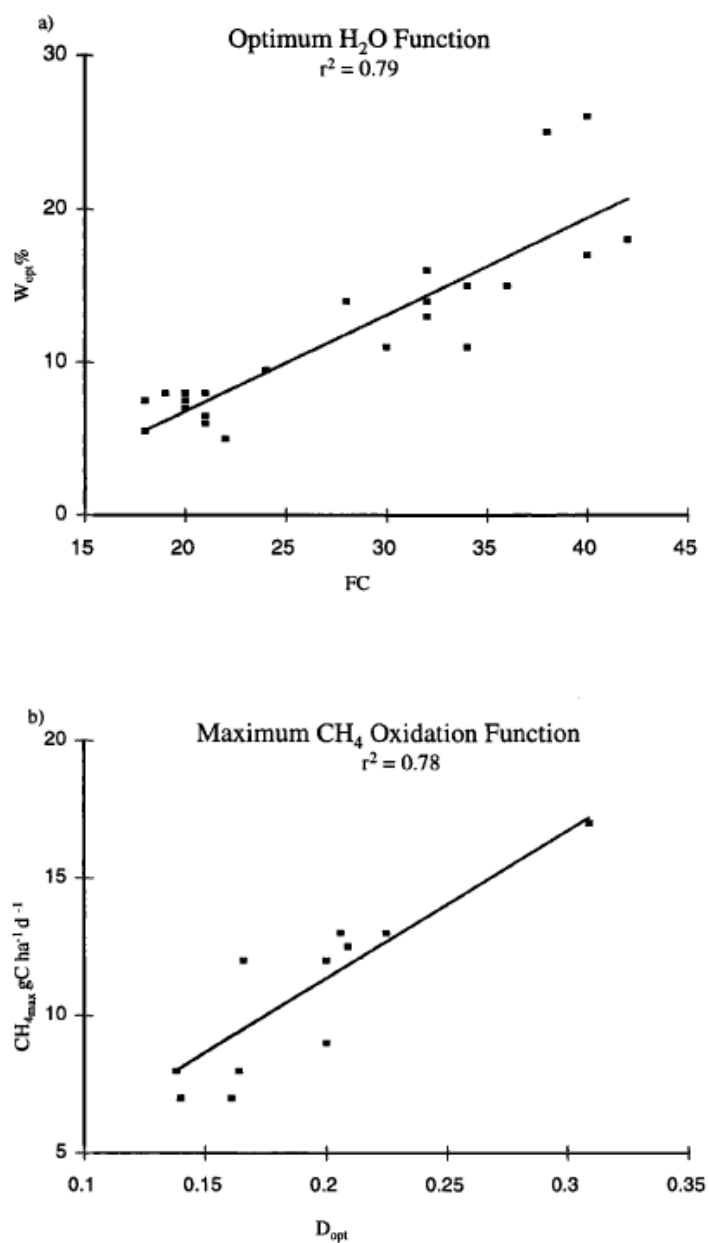**Figure 2 from Del Grosso et al. (2000b):**

Figure 2. Model parameters related to soil properties: (a) optimum water content for CH_4 oxidation as a function of field capacity (W_{opt}) and (b) maximum CH_4 oxidation rate as a function of soil gas diffusivity calculated at optimum water (D_{opt}).
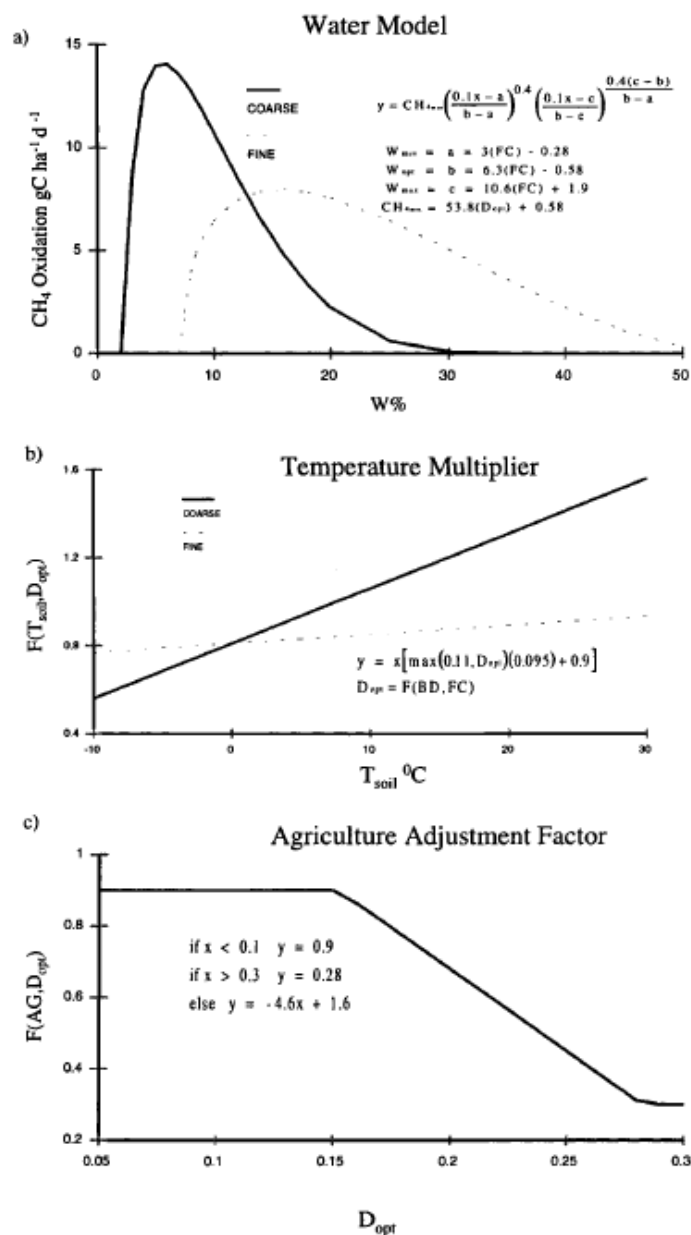
Figure 5 from Del Grosso et al. (2000b):

Figure 5. Grassland-Tropical-Coniferous forest submodel (a) CH₄ oxidation rate as a function of soil volumetric water (*W*), field capacity (FC), and gas diffusivity (*D*ₒₚₜ). (b) Multiplier accounting for the interaction between soil gas diffusivity and temperature. (c) Effect of cultivation on CH₄ oxidation rates.
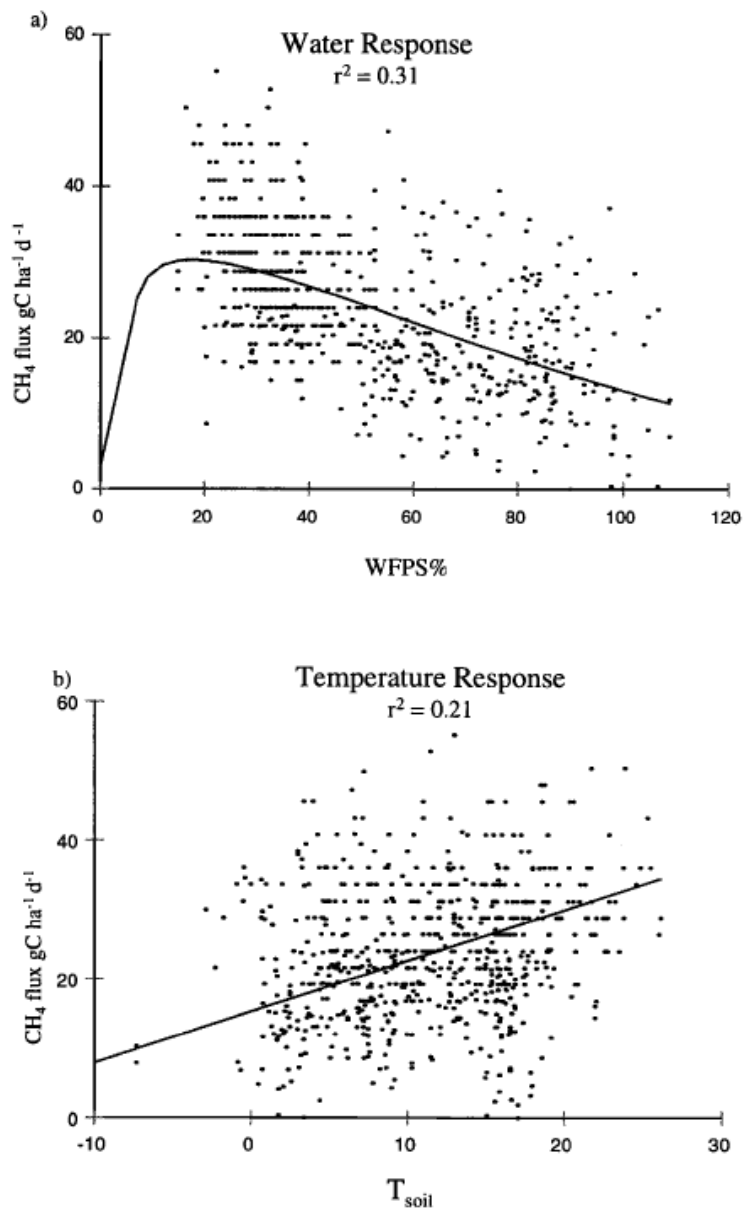
Figure 6 from Del Grosso et al. (2000b):

Figure 6. Response of CH_4 oxidation by deciduous forest soils to (a) soil water-filled pore space and (b) soil temperature.
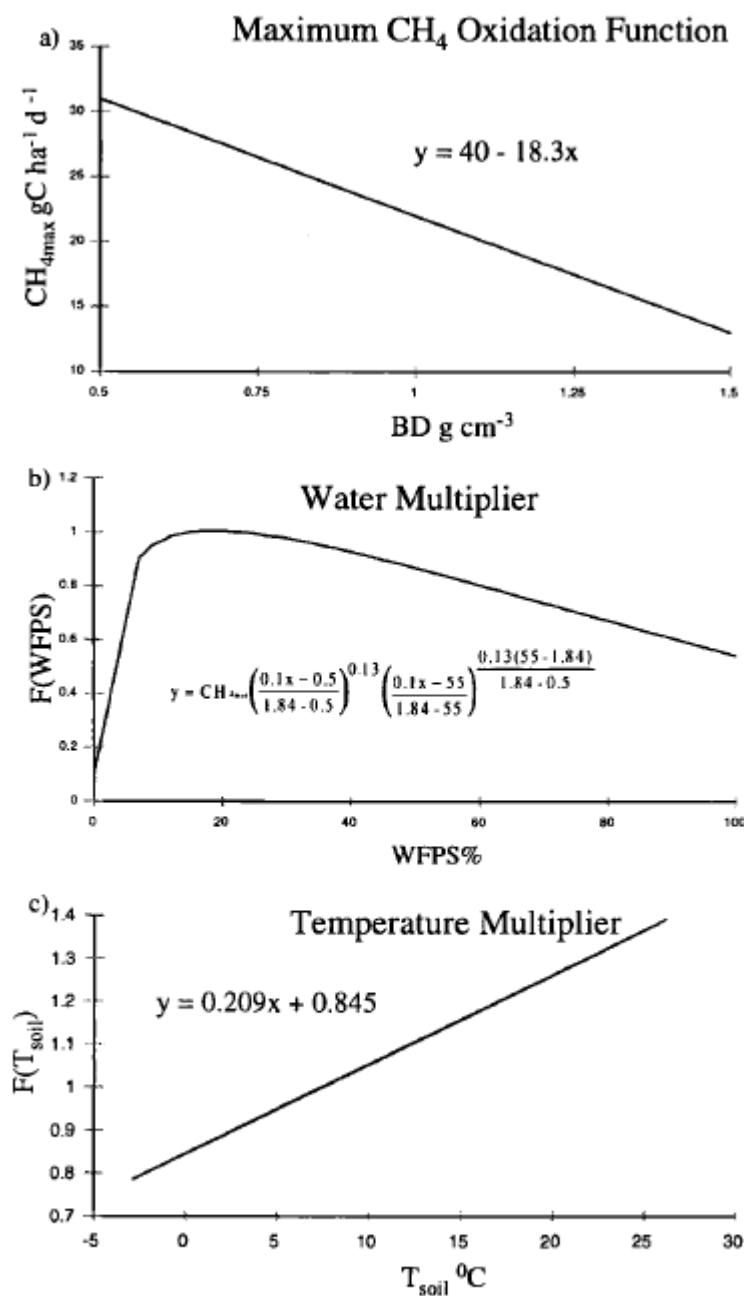
Figure 7 from Del Grosso et al. (2000b):

a) Maximum CH$_4$ Oxidation Function

$$y = 40 - 18.3x$$

(y-axis: CH_{4max} gC ha^{-1} d^{-1}; x-axis: BD g cm^{-3})

b) Water Multiplier

$$y = CH_{4m} \left(\frac{0.1x - 0.5}{1.84 - 0.5}\right)^{0.13} \left(\frac{0.1x - 55}{1.84 - 55}\right)^{\frac{0.13(55 - 1.84)}{1.84 - 0.5}}$$

(y-axis: F(WFPS); x-axis: WFPS%)

c) Temperature Multiplier

$$y = 0.209x + 0.845$$

(y-axis: F(T$_{soil}$); x-axis: T$_{soil}$ ^{0}C)

Figure 7. Deciduous Forest submodel. (a) Maximum CH$_4$ oxidation rate as a function of mineral soil bulk density. Response of CH$_4$ oxidation rate to (b) soil water-filled pore space (WFPS), and (c) soil temperature.

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