# **Chapter 13**Simulation Processes for the Nitrogen Loss and Environmental Assessment Package

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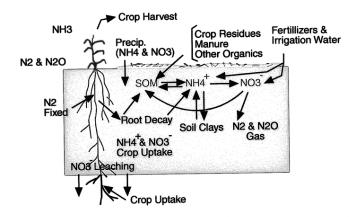
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#### NLEAP SIMULATION OF CARBON AND NITROGEN CYCLING

NLEAP simulates soil carbon and nitrogen ratio (C/N) processes for upland soils in one dimension starting with residue cover on the soil surface and continuing down through the crop root zone to the bottom of the soil profile (Figure 1). Processes include infiltration and transport of soil water and nitrates; carbon and nitrogen cycling and transformations on the soil surface and within the soil profile; surface

runoff of water, nitrate, and ammonium; nitrate leaching from the root zone; crop uptake of nitrate and ammonium; denitrification losses (including  $N_2$  and  $N_2$ O); and ammonia volatilization.

As with the previous version, NLEAP DOS the user supplies the expected crop yields, and the information is used to distribute crop uptake of water and nitrogen over the growing season. The current NLEAP can handle a wide range of agricultural crops (over 50), and additional crops can be easily configured for inclusion. The model allows for the flexibility to add crop varieties that are used at site-specific regions of the country.



# Nitrogen Cycle (upland soils)

Figure 1. The NLEAP modeling approach provides a fast and efficient means of integrating management effects with soil and climate information to calculate nitrogen (N) losses from agricultural fields. These losses include  $NO_3$ -N leaching from the crop root zone, gaseous emissions of  $N_2O$  and  $N_2$ ,  $NH_3$  volatilization, and surface wash-off of N (Shaffer and Ma, 2001).

# SUBMODELS FOR C/N CYCLING PROCESSES ON THE SOIL SURFACE AND WITHIN THE SOIL PROFILE

A submodel has been added for C/N cycling on the soil surface. This simulation accounts for decomposition of crop residues, manure, other organics, and inorganic nitrogen fertilizers that are applied to the soil surface. Decay of standing, dead crop residues is handled separately from flat-lying residue decay, and an algorithm is included to convert values of standing to flat-lying residues. The surface submodel also accounts for denitrification and gaseous losses of  $NH_3$  plus surface runoff of  $NH_4$ -N and  $NO_3$ -N.

A similar, related submodel for residue decomposition and cycling within the soil profile uses most of the base rate equations and computer code but includes different process rate coefficients and stress functions. With both submodels, individual applications of organic materials are tracked from the time they enter the soil surface or soil profile until they become soil organic matter (SOM). SOM formed on the soil surface is assumed to be part of the upper-most (Ap) soil horizon. Tillage incorporates surface materials into the soil and infiltration of water moves  $NO_3$ -N into the soil.

#### Mineralization of Soil Organic Matter

Mineralization of SOM is simulated using a two-pool model, containing a fast, readily decomposable pool and a slower humus pool (Figure 2). Decomposition within each pool is simulated using a first order rate equation of the form shown in the following equation:

$$NOMR = k_{omr} * SOM * TFAC * WFAC * ITIME * 0.58/10,$$
 (1)

where NOMR = the ammonium-N mineralized (kg/ha/time step);  $k_{omr}$  = the first order rate coefficient (fast or slow pool); SOM = soil organic matter (kg/ha); and ITIME = the size of the time step (days).

The fraction of carbon in the SOM is 0.58 and the C/N ratio is 10. Factors for temperature stress (TFAC) and water stress (WFAC) are calculated using the relationships described below. Transfer from the fast to slow organic matter pools is accomplished using a transfer coefficient, which is controllable by the user.

## NLEAP mineralization portion of C/N cycle

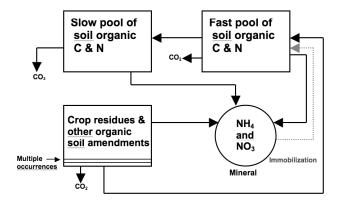


Figure 2. Mineralization of soil organic matter is simulated using a 2-pool model containing a fast, readily-decomposable pool and a slower humus pool.

#### Crop Residue and Other Organic Matter Mineralization

Mineralization of crop residues and other organic materials, such as manure, are computed using the following equations:

$$CRES = fr * RES, (2)$$

where CRES = the carbon content of the residues (kg/ha); RES = the dry residues (kg/ha); fr = the carbon fraction of the residues;

constrained by

$$CRESR = k_{res} * RADJST * CRES * TFAC * WFAC * ITIME,$$
 (3)

where CRESR = the residue carbon metabolized (kg/ha/time step);  $k_{resr}$  = the first order rate coefficient (day<sup>-1</sup>); RADJST = the rate adjustment factor depending on the current C/N ratio.

RADJST is set to 0.29 at a C/N of 100; 0.57 at a C/N of 40;1.0 at a base C/N of 25; and 2.6 at a C/N of 9. Linear interpolation is used between these points. Transfer of decayed residue material to the fast  $N_0$  pool occurs at a C/N ratio of 6.5 for manure and other organics, at a C/N ratio of 10 for crop residues starting at less than 25, and at a C:N ratio of 12 for crop residues starting at  $\geq$ 25.

The residue carbon is updated after each time step using the following equation:

$$CRES = CRES - CRESR, (4)$$

constrained by CRESR  $\leq$  CRES.

Net mineralization-immobilization is determined using the following:

$$NRESR = CRESR * (1/CN - 0.0333),$$
 (5)

constrained by

- NRESR 
$$\leq$$
 NAF + NIT1, when NRESR  $<$  0.0,

where NRESR = the net residue-N mineralized (kg/ha/time step); CN = the current carbon to nitrogen ratio of the residues used in equation 5; NAF = the ammonium-N content; NIT1 = the nitrate-N content of the top 30 cm (kg/ha).

The  $\tilde{N}$  content of the decaying residues is updated after each time step using the following:

$$NRES = NRES - NRESR, (6)$$

constrained by

NRESR < NRES.

A new value for CN is computed for the next time step using equation 7:

$$CN = CRES/NRES$$
, (7)

where NRES = N content of the crop residues, manure, or other organic wastes (kg/ha).

The mineralization of manure and other organic wastes is calculated using the same basic equation set for crop residues given above, with manure or organic wastes substituted for crop residues.

Equations 2 through 7 assume (1) that crop residues contain a user-supplied percent carbon (manure and other organic wastes are assigned percentages based on separate user-supplied analysis), (2) that net mineralization/immobilization equals zero at a C/N value of 30, and (3) that the C/N value for soil microbes is 6.0. The values of corresponding first order rate coefficients ( $k_{resr}$ ,  $k_{manr}$ , and  $k_{othr}$ ) depend on the material being decomposed and the current C/N values. In general, fresh materials are assigned a higher rate coefficient until a C/N value is reached, where most of the faster pool has been decomposed and a lower rate coefficient is required.

In the case of surface standing dead crop residues, a conversion function is used to estimate when standing residues break off and become flat-lying on the ground. This function is driven by decay of the residue base, wind run, and tillage and can be expressed as follows:

$$RESMOV = k_{till} * (1 - RES/SSORIG) * WINDRUN/250000,$$
 (8)

where RESMOV = the daily fraction of the standing residue converted to flatlying;  $k_{till}$  = a tillage coefficient (0.045 with tillage, 0.035 without tillage); RES (kg/ha) = the mass of residue contacting the soil; SSORIG (kg/ha) = the mass of original fresh residue contacting the soil; WINDRUN (km) = total wind since the residue was fresh.

# Nitrification and N<sub>2</sub>O Emissions

The nitrification of ammonium-N is calculated using the following equation:

$$N_n = k_n * TFAC * WFAC * ITIME,$$
(9)

constrained by

$$N_n \leq NAF$$
,

where  $k_n$  = the zero order rate coefficient for nitrification (kg/ha/time step); TFAC = the temperature stress factor (0-1); WFAC = the soil water stress factor (0-1); ITIME = the length of the time step (days); NAF = the ammonium-N content of the top 30 cm (kg/ha).

The use of nitrification inhibitors is simulated by reducing the magnitude of the rate coefficient,  $k_n$ .  $N_2O$  emissions ( $NN_{N2O}$ ) from the nitrification process are computed using the equation:

$$NN_{N2O} = N_n * alpha * TFAC * WFAC,$$
 (10)

where alpha = the maximum fraction of  $N_2O$  leakage from the nitrification process when temperature and water content are not constraining factors.

# Losses to Denitrification ( $N_2$ plus $N_2O$ )

Nitrogen lost to denitrification ( $N_{det}$ ) during the time spans ending with precipitation and irrigation events is computed using the equation:

$$N_{det} = k_{det} * NIT1 * TFAC * [NWET + WFAC * (ITIME - NWET)],$$
 (11)

constrained by

$$N_{det} < NIT1$$
,

where  $N_{det}$  = nitrate-N denitrified (kg/ha/time step);  $k_{det}$  = the rate constant for denitrification; NIT1 = the nitrate-N content of the top 30 cm (kg/ha); NWET = the number of days with precipitation or irrigation during the time step (for daily time steps NWET is either 1 or 0).

The value assigned to  $k_{\text{det}}$  is a function of percent SOM, soil drainage class, type of tillage, presence of manure, tile drainage, type of climate, and occurrence of pans (Meisinger and Randall, 1991). Equation 11 offers the ability to calculate maximal denitrification occurring on the wet days, while calculating a separate estimate of denitrification under dryer soil water conditions for other days.

N<sub>2</sub>O emissions from denitrification are calculated based on extensions to equation 11 (Xu et al., 1998). Emissions for wet conditions are calculated using the following equation:

$$NW_{N2O} = N_w^* \text{ alpha}_w, \tag{12}$$

where  $N_w$  = total nitrogen denitrified under wet conditions; alpha<sub>w</sub> = the fraction of total N denitrified as  $N_2O$  under wet conditions.

For dry soil conditions, N<sub>2</sub>O emissions are estimated using the following equation:

$$ND_{N2O} = N_d^* alpha_d^* (1 - WFAC), \qquad (13)$$

where  $N_d$  = total nitrogen denitrified under dry conditions; alpha<sub>d</sub> = the maximum fraction of total N denitrified as  $N_2O$  at 50 percent water-filled pore space.

Total  $N_2O$  emissions ( $N_{N2O}$ ) are then calculated as a sum of the components:

$$N_{N2O} = NN_{N2O} + NW_{N2O} + ND_{N2O}. (14)$$

 $N_2$  gas emissions are calculated by subtracting  $N_{N2O}$  from  $N_d$ .

#### Temperature Stress Factor

The soil temperature stress factor, TFAC, is computed using an Arrhenius equation of the form:

$$TFAC = 1.68E9 * EXP (-13.0/(1.99E-3 * (TMOD+273))),$$
 (15)

where TMOD = (T - 32)/1.8 when  $T \le 86$ °F; TMOD = 60 - (T - 32)/1.8 when T > 86°F (T is soil temperature in °F).

TFAC has a range of 0.0 to 1.0. This equation was developed using data reported by Gilmour (1984) and Marion and Black (1987). Equation 15 approximately doubles the rate for each 18°F increase in soil temperature below a maximum of 86°F and halves the rate for equivalent increases above 86°F.

The above equations for TFAC apply to the soil simulation model only. TFAC for use on the soil surface is calculated using a modified version of the soil equations.

#### Soil Water Stress Factor

The soil water factor, WFAC (also range 0.0 to 1.0), is computed as a function of percent water-filled pore space (WFP) by using curves fitted to data developed by Linn and Doran (1984) and Nommik (1956) for aerobic and anaerobic processes. For aerobic processes such as mineralization and nitrification, the following equations are used:

WFAC = 
$$0.0075 * WFP$$
, (16)

where WFP  $\leq$  20;

$$WFAC = -0.253 + 0.0203 * WFP,$$
 (17)

where  $20 \le WFP < 59$ ;

WFAC = 
$$41.1 * EXP(-0.0625 * WFP)$$
, (18)

where WFP  $\geq$  59; and

$$WFAC = 0.000304 * EXP(0.0815 * WFP),$$
(19)

for anaerobic processes such as denitrification.

The above equations for WFAC apply to the soil simulation model only. WFAC for use on the soil surface is calculated using a modified version of the soil equations.

#### Crop N Uptake

Nitrogen taken up by the crop  $(N_{\text{plt}})$  is calculated using the following equations:

$$N_{dmd} = YG * TNU * fNU * ITIME,$$
 (20)

where  $N_{dmd} = N$  uptake demand (kg/ha/time step); YG = yield goal or maximum yield in appropriate units; TNU = total N uptake (kg/harvest unit); fNU = fractional N uptake demand at the midpoint of the time step.

A normalized curve relating fNU to relative crop growth stage is used to proportion N uptake demand (Shaffer et al., 1991). The N uptake demand is proportioned between the upper and lower soil horizons according to the relative water uptake. N available for uptake in each horizon is computed as follows for the upper horizons:

$$Navail_1 = NAF + NIT1, (21)$$

and as follows for the second and third horizons:

$$Navail_{2or3} = NIT2 \text{ or NIT3}, \qquad (22)$$

where NIT2 or NIT3 = the nitrate-N contents in the lower horizons (kg/ha). Note that a third horizon has been added as follows:

$$Navail_3 = NIT3$$
 (23)

This three-horizon configuration provides the same capability as that provided by NLEAP version 1.2, reported by Delgado et al. (1998).

In each case, the uptake demand for each layer is constrained by the nitrogen availability. Therefore,  $N_{plt}$  is set equal to the smaller of  $N_{dmd}$  or  $(Navail_1 + Navail_2 + Navail_3)$ . Plant uptake of ammonium-N (NPLTA) is calculated from total N uptake in the upper 30 cm according to the fraction of nitrate-N plus ammonium-N that is ammonium-N.

#### Soil N Uptake by Legumes

Soil nitrogen uptake by legumes is considered to be the lesser of either the nitrogen demand by the crop or the sum of Navail<sub>1</sub> + Navail<sub>2</sub> + Navail<sub>3</sub>. If the nitrogen demand is greater than the nitrogen available in the soil, it is assumed that the plant obtains the difference from nitrogen fixation.

#### N Loss to Ammonia Volatilization

Nitrogen lost to ammonia volatilization ( $N_{NH3}$ ) during the same time steps discussed above is calculated using the following equation:

$$N_{NH3} = k_{af} * NAF * TFAC * ITIME,$$
 (24)

constrained by

 $N_{NH3} \leq NAF$ ,

where  $N_{NH3}$  = ammonia-N volatilized (kg/ha/time step);  $k_{af}$  = the rate constant for ammonia volatilization; NAF = the ammonium-N content of the top 30 cm (kg/ha).

The particular value used for  $k_{af}$  is a function of fertilizer application method, occurrence of precipitation, cation exchange capacity of surface soil, and percent residue cover (Meisinger and Randall, 1991). In the case of manure,  $k_{af}$  is a function of the type of manure and application method (Meisinger and Randall, 1991).

#### Water Available for Leaching

Water available for leaching (WAL) is calculated after each precipitation and irrigation event using the three-horizon soil model and the following equations:

WAL1 = 
$$P_e$$
 - ET1 - (AWHC1 -  $S_{t1}$ ), (25)

constrained by

WAL1 > 0.0, and

$$WAL2 = WAL1 - ET2 - (AWHC2 - S_{12}),$$
 (26)

$$WAL3 = WAL2 - ET3 - (AWHC3 - S_{13}),$$
 (27)

constrained by

 $WAL \ge 0.0$ ,

where WAL1 = water available for leaching from the top 30 cm; WAL2 and WAL3 = water available for leaching from the second and third horizons (cm); ET1 and ET2 = potential evapotranspiration associated with the top two horizons (cm/time step); AWHC1 and AWHC2 = the available water holding capacities of the upper two horizons (cm); WAL = water available for leaching from the bottom of the soil profile (cm);  $P_e$  = effective precipitation (inches); ET2 and ET3 = potential evapotranspiration from the lower two horizons (cm);  $S_{t1}$  = available

water in the top 30 cm at the end of the previous time step (cm); AWHC2 and AWHC3 = available water holding capacities of the second and third horizons (cm);  $S_{t2}$  and  $S_{t3}$  = available water in the lower two horizons at the end of the previous time step.

#### Potential Evapotranspiration

Potential evapotranspiration is computed using pan evaporation data and appropriate coefficients as follows:

$$ET_{p} = EV_{p} * k_{pan} * k_{crop} * ITIME,$$
(28)

where  $ET_p$  = potential evapotranspiration (cm/time step);  $EV_p$  = average daily pan evaporation during the time step (cm/day);  $k_{pan}$  = pan coefficient;  $k_{crop}$  = crop coefficient.

 $\mathrm{ET_p}$  is proportioned between potential evaporation at the soil surface ( $\mathrm{ET_{ps}}$ ) and potential transpiration ( $\mathrm{ET_{pt}}$ ), using normalized curves for each crop.  $\mathrm{ET_{pt}}$  is then proportioned between the upper and lower soil horizons according to the relative root distributions. Actual surface evaporation for any time step is considered to be the lesser of either  $\mathrm{ET_{ps}}$  or the soil water available for evaporation. Actual transpiration for each time step and soil horizon is considered to be the lesser of either the potential transpiration for that layer or the remaining soil water above the permanent wilting point. If one horizon is depleted of water, an attempt is made to extract the water from the next horizon.

#### Nitrate-N Leached

Nitrate-N leached (NL (kg/ha)), during a time step is computed using an exponential relationship (Shaffer et al., 1991), expressed as follows:

$$NL1 = NAL1*(1 - exp(-1.2*WAL1/POR1)),$$
 (29)

$$NAL2 = NAL2 + NL1, (30)$$

$$NL2 = NAL2*(1 - exp(-1.2*WAL2/POR2)),$$
 (31)

$$NAL = NAL3 + NL2, (32)$$

$$NL = NAL^*(1 - exp(-1.2*WAL/POR3)),$$
 (33)

where NL1 and NL2 = nitrate-N leached from the top two horizons (kg/ha); POR1 = the porosity of the top 30 cm (cm); POR2 = the porosity of the second horizon (cm); NAL1, NAL2, and NAL3 = the nitrate-N available for leaching at the start of the time step for each horizon (kg/ha); NAL = nitrate-N available for leaching from the root zone (kg/ha); NL = nitrate-N leached from the bottom of the root zone (kg/ha); POR3 = the porosity of the lower horizon (cm).

Total nitrate-N leached for any month or year is computed by summing the leaching values obtained from each time step during the period of interest.

#### **SUMMARY**

The identification of potential problems with N losses quickly leads to a list of potential solutions in terms of BMPs. Local Extension and USDA Natural Resources Conservation Service have identified practices shown to be of value in each local region. This list should be used as a starting place and potential BMPs evaluated for the site-specific conditions. Some common practices for control of NO<sub>3</sub>-N leaching include multiple fertilizer applications, the use of fall cover crops to recover residual soil NO<sub>3</sub>-N, adjustment of fertilizer and manure rates to account for other sources of N, precision application of fertilizers across a field, use of management zones, crop rotations with deeper rooted crops and legumes, and avoidance of off-season fertilizer applications. The relative effectiveness of each method will depend on site-specific conditions and can be evaluated by comparing simulated N loss results with corresponding results using the historical data. NLEAP has been used to evaluate BMPs across several different regions, agroecosystems, and climates.

There is potential to use NLEAP as a management tool to assess the effect of BMPs. The NLEAP model uses national database resources from soils, climate, and management, which allows for the potential application of the model without any ground-truthing. We caution the users to be aware that application of the model without a previous evaluation of local conditions and management are often wrong, leading to a poor application of the model and questionable results.

We emphasize that the users and staff should visit the site; talk to local producers, USDA Natural Resources Conservation Service, and Extension; and take some samples if possible. Users need to remember that N losses (especially their magnitudes) are often determined by local effects, as opposed to regional or national generalizations. Users need to review Shaffer and Delgado (2001) and Delgado and Shaffer (2008) and their recommendation for a Tier approach to management. If more detailed and accurate results are needed, users should move to a tier 3 approach, supported by research at the local site. The model will use adequate databases, accurate information, and realistic management scenarios that have been calibrated and evaluated only when examples can be reported by multiple national and international users across hundreds of simulations.

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