

ENVIRO-GRO User Manual

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The present ENVIRO-GRO model evolved from concepts of John Letey and the computer programming and simulations conducted by associates. In close cooperation with John Letey, Dr. Peter Vaughan developed the new version of the ENVIRO-GRO program and produced all computational and graphical materials appearing in this document.

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Preface

The ENVIRO-GRO program existed in two versions prior to the current work. The original ENVIRO-GRO, developed in the 1990s, was a Fortran program incorporating some earlier numerical codes of Nimah and Hanks (1973) and van Genuchten (1987) that solved the Richards equation and the convection-dispersion equation. A later version of the program was written in the 2000's that included a graphical user interface. This version used a Runge-Kutta numerical solution of solute transport and a modified WatFlow subroutine for calculation of water flow (Simunek et al., 1996). This version had significant performance problems due to the excessive resource requirements of the graphical interface.

The present version of ENVIRO-GRO was created to address issues associated with both the original code and the GUI-interface version. The contract with Dr. Peter Vaughan for development of the new code specified that the code would be a standard Fortran 77 program which accepted input in the form of text files and produced text file output. No GUI-interface was created partly because of the performance problems encountered in the earlier version but also because the contractor believes that a GUI-interface for these kinds of programs is not the most efficient way to do production-level simulation work. Such interfaces require the user to navigate through many data-entry screens to complete a single run when many real-world problems require numerous runs that have only minor variations in the complete input datasets. The use of scripting languages like Perl to generate sets of input data files and shell languages to execute ENVIRO-GRO and store output files can be a more efficient way to address problems requiring many runs of the program.

ENVIRO-GRO is meant to be used primarily for simulations of the production of agricultural crops and associated water quality issues. The standard units are length (cm), time (days) and mass (kg/ha). Thus, irrigation events would be specified as an application rate in cm/day. Although the main time unit is days, boundary conditions can be changed for periods shorter than one day allowing simulations for higher frequency irrigation events or hourly changes in potential evapotranspiration. The present version of ENVIRO-GRO was designed to be substantially more efficient than the prior version with the GUI-interface. A simulation of 15 consecutive seasons of corn with organic fertilization events took less than a minute to run on a 64-bit AMD E-350 dual-core processor.

The version of ENVIRO-GRO produced in 1998 featured a nitrogen module that included nitrate transport, fertilization with inorganic nitrogen, fertilization with organic nitrogen incorporated into the soil by tillage, mineralization of organic nitrogen through a standard decay process and root uptake of nitrogen with compensation. Simulation of each of these processes was built into the new program and these reprogrammed simulations adhere precisely to the original descriptions (Pang and Letey, 1998).

The sensitivity of plant root water uptake to matric and salinity stresses has always been an essential part of ENVIRO-GRO. The algorithms for calculation of root water uptake were reprogrammed in the present version but the same features were maintained. These include use of the additive formulation for calculation of the root water uptake reduction factor for combined matric and osmotic stresses (Pang and Letey, 1998) and the calculation of the compensation

effect when portions of the root zone are unstressed. Oster et al.(2012) included ENVIRO-GRO in a comparison of features and simulated results with several other transient-state models that account for matric and osmotic effects on crop production. None of the other models allow nitrogen effects to be included.

This manual describes the mathematical representations of processes that are simulated by ENVIRO-GRO. Subsurface water flow is the central process that includes the physics of water flow through a variably-saturated porous medium and the sink for water that is root system of plants. Chemical transport is the process whereby salts and nitrate move vertically in the soil profile as a consequence of water flow. Both convection and dispersion are represented in the chemical transport calculation. The manual contains sections describing salt and nitrate transport and the other processes affecting nitrate that were mentioned above. In order to use a console application such as ENVIRO-GRO the user must understand how the input data are arranged among the various input files so the manual explains this in detail with examples. Also, the output files are discussed in a separate chapter. Three examples of the use of ENVIRO-GRO for studying problems of varying levels of complexity are presented. The last chapter provides some advice on setting up and running the executable program.

A pesticide module can be added to ENVIRO-GRO to simulate pesticide transport through soil as reported by Pang and Letey (1999). The pesticide module is not included in the present version.

Introduction

Developments in the numerical solution of subsurface water flow and chemical transport in the 1970s and 1980s provided the possibility of developing transient-state models that had more realistic representation of boundary conditions, soil hydraulic properties and root water uptake than had been possible using steady-state models. ENVIRO-GRO was first developed as a one-dimensional, transient-state model of subsurface water flow and chemical transport specifically designed for agricultural applications (Cardon and Letey, 1992a,b,c). The model provided predictions of relative yield for crops and considered stress effects on plant growth caused by matric and salinity stress.

A major modification of ENVIRO-GRO was the introduction of nitrate transport and nitrogen uptake by plants (Pang and Letey, 1998). This version of the program also handled the production of nitrate through mineralization of organic nitrogen. A significant feature of the program allowed additional water or nitrogen to be taken up from unstressed portions of the root zone to compensate for reductions in uptake from stressed portions of the root zone. Consistent with research findings, the simulated uptake is equal to potential uptake until the entire root zone is stressed.

The original water flow and chemical transport modules were based on computer programs developed by Nimah and Hanks (1973) and van Genuchten (1987). The interfacing of these codes resulted in a complicated program that had some duplication of functions. Thus, the development of a new version of ENVIRO-GRO was undertaken to simplify the representation water flow and chemical transport with a more standardized approach and a reprogramming of the features of ENVIRO-GRO to provide greater reliability and access by the user.

The ENVIRO-GRO program simulates subsurface variably-saturated water flow, solute transport, root water uptake, N uptake, and relative yield for agricultural applications. The water flow calculations are based on numerical solution of the Richards equation and solute transport is represented by the convection-dispersion equation. Potential root water uptake as a function of depth is calculated from the total potential transpiration multiplied by a function of root density. The stress effect on root water uptake due to salinity and drought is a reduction function in which both salinity and matric stress are included in an additive formulation (Pang and Letey, 1998). This reduction function multiplies the potential root water uptake to obtain actual root water uptake. Root water uptake may be further modified by a compensation function that removes water from less-stressed depth ranges to compensate for reduced uptake elsewhere. Relative yield is calculated as the ratio of total actual root water uptake during a cropping season to the total potential root water uptake.

Inorganic nitrogen is either in the nitrate (NO_3) or ammonium (NH_4) form. Plant uptake is relatively insensitive to the form of N. However, the transport is affected with nitrate being completely mobile and ammonium being less mobile because of bonding with negatively charged soil. Nitrogen undergoes very complex transformations in the soil. In order to keep the model manageable it was assumed that nitrification was rapid so that all inorganic N was NO_3 . Denitrification and immobilization, other than plant uptake, were assumed to be negligible. A consequence of these assumptions is that the simulated NO_3 transported beyond the root zone represents the maximum amount and the actual amount may be less.

Transport of NO_3 , a conservative tracer species and salt is calculated by the program. $\text{NO}_3\text{-N}$ can be applied at the soil surface through fertigation by specifying a nitrate concentration in irrigation water. Alternatively, the program provides for fertilization events when nitrate can be incorporated into layers in the soil that are defined by the user. Another source of $\text{NO}_3\text{-N}$ is due to mineralization of organic matter. This process is also represented by a modified exponential decay model described in the section entitled “Nitrogen Source”. The application of organic nitrogen fertilizers can also be specified for fertilization events. Potential root uptake of $\text{NO}_3\text{-N}$ is prescribed by the user and the relative N uptake is provided in the “CropFinal.dat” output file.

ENVIRO-GRO offers two choices of lower boundary condition. The simplest case is free drainage which is specified by setting a Boolean variable in the “Basic.in” file to “True”. Free drainage means that the spatial derivative of the hydraulic head is equal to unity at the lower boundary. The free drainage condition is a good representation of a deep water table. It is important that the bottom boundary be placed well below the root zone where a unit hydraulic gradient is expected to exist. The other case is prescribed head which can be used to simulate conditions of a shallow water table. The prescribed head values are entered in the “Bound.in” file.

The model inputs must be specified using commonly-accepted metric units for agricultural model calculations. The input data are contained in ten input files. These files should be included together in a working folder for a particular simulation. Many of the kinds of problems that could be analyzed using ENVIRO-GRO involve varying just a few of the input variables. The choice to have more files rather than a single file with a complicated format was made to simplify the data file preparation for these kinds of situations. The output data are stored in the working folder in twelve output files having the suffix (.dat). These are standard text files that can be opened in a word processor or a spreadsheet. The most important file contains the path to the current working directory. This path must be stored in the “datPath.txt” file that is located in the same folder as the data files that will be accessed by ENVIRO-GRO program. Further details concerning the installation and operation of the program are contained in the final chapter of this manual.

Water Flow for Variably-saturated Conditions

Governing Equation

Water flow is represented in ENVIRO-GRO by a numerical solution of the Richards equation (Pang and Letey, 1998).

$$\frac{\partial \theta_w}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial h}{\partial z} + 1 \right) \right] - S \quad (2.1)$$

This equation expresses the one-dimensional flow of water within a variably-saturated porous medium such as soil. The volumetric water content, θ_w , varies due to the water flux given by the first term on the right side and the sink term, S . The units of the equation are inverse days (d^{-1}). h is the pressure head (cm) and K is the hydraulic conductivity ($cm\ d^{-1}$). The equation is non-linear because K varies as a function of h . The solution of the equation requires specification of the functional relationship between θ_w and h known as the water retention function.

The water content of a soil decreases with decreasing pressure or matric head (h) such that a matric head of zero represents a water-saturated soil ($\theta = \theta_s$). For dry conditions the matric head has large negative values as the water content approaches the residual water content ($\theta = \theta_r$).

The functional relationship of θ and h is:

$$\theta(h) = \begin{cases} \theta_r + \frac{\theta_s - \theta_r}{\left[1 + |\alpha h|^n \right]^m} & h < h_s \\ \theta_s & h \geq h_s \end{cases} \quad (2.2)$$

Matric heads greater than or equal to the matric head at saturation (h_s) correspond to saturated water content (θ_s). For matric heads less than h_s the water content varies between the residual water content (θ_r) and θ_s (Mualem, 1976; van Genuchten, 1980). The parameters of equation (2.2) are α (cm^{-1}), m and n . A common assumption, used in ENVIRO-GRO, is the relationship: $m = 1 - 1/n$ (van Genuchten, 1980). These parameters plus the saturated and residual water content are material properties of soils that must be specified by the user. For example, material properties for Panoche clay-loam generated a typical sigmoidal curve when plotted against the logarithm of matric head (Fig. 1).

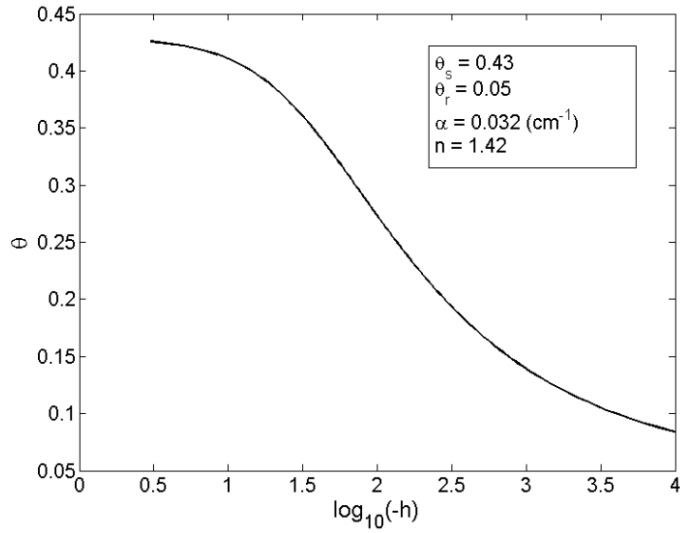


Figure 1. Retention curve for Panoche clay-loam.

Variation of hydraulic conductivity with matric head is the product of the saturated hydraulic conductivity (K_s) and a factor (K_r) (van Genuchten, 1980):

$$K(h) = \begin{cases} K_s & h > h_s \\ K_s K_r(h) & h \leq h_s \end{cases} \quad (2.3)$$

$$K_r = \sqrt{S_e} \left[1 - \left(1 - S_e^{1/m} \right)^m \right]^2 \quad (2.4)$$

where S_e is the scaled water content:

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (2.5)$$

The saturated hydraulic conductivity and the four water retention parameters comprise the soil hydraulic properties specified for each soil layer.

Root Density Distribution

Root water uptake, at a specified depth, is represented as the product a root density distribution, a potential root water uptake distribution and various stress functions. The root density distribution is a trapezoidal function which is unity near the soil surface and decreases linearly below one-third of the current rooting depth (Fig. 2). The depth at which the linear decrease begins was

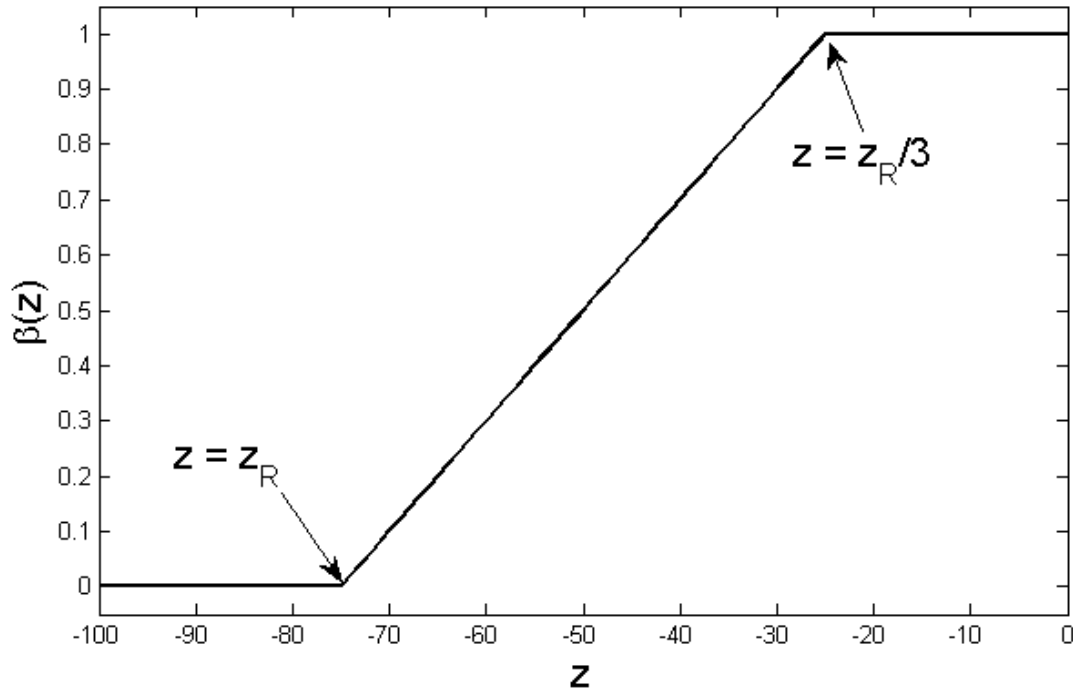


Figure 2. Root density function.

determined from the assumption that one-half of the root water uptake will occur above that depth and the remainder below. The expression for the root density distribution is:

$$\beta(z) = \begin{cases} 1 & z \geq z_R/3 \\ 3 - 3(z + z_R)/(2z_R) & z_R \leq z < z_R/3 \\ 0 & z < z_R \end{cases} \quad (2.6)$$

The current rooting depth is z_R . Depth at the soil surface is assumed to be zero and depths below the surface are negative. Allowing water or N uptake to equal potential uptake until the entire root zone is stressed largely mitigates the effects of prescribing a root zone distribution that differs from the true distribution.

Root Water Uptake

Potential root water uptake as a function of depth for a non-stressed condition is determined by multiplying the root density function by the potential transpiration. The transpiration can be calculated as the depth integral of the root water uptake:

$$T = T_p \int_{L_R}^0 \beta(z) dz \quad (2.7)$$

For non-stressed conditions $T=T_p$ implying that the depth integral of β must be unity. Transpiration calculations of the type represented by (2.7) therefore require that β be normalized.

Stress conditions for root water uptake include salinity and matric stresses. The salinity and matric stress effects are represented by a combined function that has a sigmoidal form (Pang and Letey, 1998).

$$\alpha_{hs} = \frac{1}{\left[1 + \left(\frac{h}{h_{50}} + \frac{\pi}{\pi_{50}}\right)^3\right]} \quad (2.8)$$

The parameters h_{50} and π_{50} are the values of matric and salinity stress which generate a 50% reduction of the stress function (α_{hs}). π is the osmotic head at depth z . Osmotic head is generated by dissolved salts in the soil water and is calculated from the solute concentration. The ENVIRO-GRO program approximates osmotic head as a linear function of solute concentration where solute concentration does not refer to some specific salt. For agricultural applications the detailed chemical analyses of irrigation waters may not be available but the total dissolved solids can be easily estimated from measurement of electrical conductivity.

The Maas-Hoffman model of crop yield reduction as a function of root zone salinity is comprised of a threshold salinity and subsequent linear reduction with increasing salinity (Maas and Hoffman, 1977). The parameters of the model are the threshold salinity and the slope of the linear function. Eq. (2.8) does not represent a true threshold because α_{hs} decreases for even small salt concentrations in the root zone. The ENVIRO-GRO model implements a true threshold by overriding the reduction factor computed by Eq. (2.8). This is accomplished by computing α_{hs} and comparing the value to a specified threshold α_t :

$$\alpha_{hs} = \begin{cases} 1 & \alpha_{hs} > \alpha_t \\ \alpha_{hs} & \alpha_{hs} \leq \alpha_t \end{cases} \quad (2.9)$$

The threshold matric head h_t is supplied by the user and the threshold osmotic head is calculated from the Maas-Hoffman threshold coefficient (Maas and Hoffman, 1977). Because plant root water uptake responds to the electrical conductivity (EC) of the soil water, the Maas-Hoffman threshold electrical conductivity is multiplied by a factor of two approximating the difference in EC for the water content of a saturated paste (EC_e) and for that of in-situ soil water content (EC_{sw}). The threshold value, α_t , is determined from these threshold values for pressure head, h_t , and osmotic head, π_t , by inserting these threshold values into (2.8) (Pang and Letey, 1998). If α_{hs} at all depths is greater than α_t , the root zone is unstressed and total root water uptake occurs at the potential value T_p . Alternatively, if $\alpha_{hs} < \alpha_t$ over the entire root zone then root water uptake is limited by α_{hs} at all depths. Finally, if the root zone is divided into both stressed and

unstressed depth ranges then root water uptake may exceed $\beta(z)T_p$ at some nodes as compensation for less root water uptake over stressed depth ranges.

Root Water Uptake for Stressed Conditions and Compensation

Transpiration for stressed conditions (T_s) is calculated using an equation similar to (2.7) that includes the stress function (α_{hs}):

$$T_s = T_p \int_{z_R}^0 \beta(z) \alpha_{hs}(z) dz \quad (2.10)$$

This method for calculating transpiration rate does not recognize the capability of plants to actively redirect root water uptake from highly-stressed zones to zones of lower stress known as compensation (Pang and Letey, 1998; Jarvis, 1989). Compensation can occur when α_{hs} varies with depth such that $\alpha_{hs}(z) < \alpha_t$ over some depth range and $\alpha_{hs} > \alpha_t$ for another depth range. The program calculates the difference in water uptake ($T_p - T_s$). For each depth increment, if $\alpha_{hs} > \alpha_t$ an amount of water is extracted to attempt make up this difference. A new value of T_s is generated and, if this value remains less than T_p , then the difference is recalculated and the process of water extraction is repeated. A limit of 15 cycles is prescribed by the program. During each cycle the pressure head and salinity for each depth increment are recalculated following the water extraction. This may cause certain depth increments to generate $\alpha_{hs} < \alpha_t$. This process of successive approximation determines the sink term S in eq. (2.1) as the difference in water content the beginning and end of a time step divided by the length of the time step.

Boundary Conditions

ENVIRO-GRO has a boundary condition at the soil surface of prescribed flux. If soil evaporation is occurring then the upward potential evaporative flux is the boundary condition. During precipitation or irrigation events the prescribed flux based on the application rate is applied. If actual infiltration rate cannot match the prescribed flux due to insufficient hydraulic conductivity then the upper boundary condition automatically switches to prescribed head and ponding of water occurs at the surface.

The lower boundary conditions may be set as free drainage or as prescribed head. The free drainage condition means that the derivative of hydraulic conductivity with respect to depth at the bottom of the profile is unity. This condition is usually applied when the water table is substantially below the bottom of the modeled profile. The prescribed head condition is available for modeling shallow water tables that may change in elevation during the period of a simulation. Prescribed pressure heads can be positive indicating that the water table is above the bottom of the profile. By varying these positive pressure heads over time, the vertical movement of the water table can be simulated.

Chemical Transport and Nitrogen Uptake

Governing Equation

Chemical transport is represented by the convection-dispersion equation (Pang and Letey, 1998):

$$\frac{\partial(\theta c_i)}{\partial t} = \frac{\partial}{\partial z} \left[D(\theta, v) \frac{\partial c_i}{\partial z} - v c_i \right] - S_i c_i + S_i^* \quad (3.1)$$

c_i is the solute concentration of species i (mmol/L) and θ is the water content. The species represented are a conservative tracer, salt and $\text{NO}_3\text{-N}$. The third term on the right hand side represents the root uptake of species i . For the tracer and salt both S_i and S_i^* are zero because root uptake and subsurface production of these species are presumed to be nil. The fourth term is a source term which represents the production of nitrate in the soil. v is the pore water velocity and θ is the water content. D is a function representing the combined effects of molecular diffusion and dispersion (Pang and Letey, 1998):

$$D(\theta, v) = D_m \xi + \lambda |v| \quad (3.2)$$

λ is the mechanical dispersivity (cm) and is multiplied by the pore water velocity, v . The molecular diffusion coefficient (D_m) is multiplied by a tortuosity factor ξ which is calculated using the Millington-Quirk model (Millington and Quirk, 1961):

$$\xi = \theta^{7/3} / \theta_s^2 \quad (3.3)$$

θ_s is the saturated water content (presumed equal to the total porosity). As an approximation, the molecular diffusion coefficient is presumed to be the same for all species.

Boundary Conditions

Either flux (Cauchy) or fixed value (Dirichlet) conditions may be applied at the soil surface or lower boundary. The Cauchy condition is prescription of the concentration flux that includes both the diffusive and convective fluxes:

$$-\theta D_i \frac{\partial c_i}{\partial z} + q_w c_i = q_w(t) c_{i0}(t) \quad (3.4)$$

The specified flux is the term on the right hand side consisting of the water flux (q_w) and the flux concentration (c_{i0}). The Dirichlet condition is

$$c_i = c_{0i}(t) \quad (3.5)$$

where the time-dependent specification of the concentration may be applied at either boundary. For the case of free drainage, the variation of concentration with depth is zero at the lower boundary:

$$\frac{\partial c_i}{\partial z} = 0$$

Nitrogen Source

Nitrate transport as modeled by eq. (3.1) requires specification of sinks and sources of nitrate. Nitrogen cycling among organic, inorganic and gaseous forms is highly complex making simplification a necessity. The ENVIRO-GRO model does not consider denitrification or immobilization within the soil. Mineralization of organic nitrogen is one source of nitrate within the soil. The present program version differs from Pang and Letey (1998) by allowing the organic material to be composed of two pools with differing decay rates. The equation for remaining organic N (N_r) is:

$$N_r(t) = (1 - \psi)N_0e^{-\lambda_1 t} + \psi N_0e^{-\lambda_s t} \quad (3.6)$$

This equation represents simultaneous decay of both a fast pool having decay coefficient λ_1 and a slow pool represented by λ_s . N_0 is the initial concentration of N in the soil (kg ha^{-1}). ψ is the fraction of N_0 that is initially present in the slow pool. Slow pool decay in ENVIRO-GRO has a fixed decay rate of 1% per year which is a common assumption for the decay rate of native organic matter in the soil ($\lambda_s = 2.75\text{E-}05 \text{ d}^{-1}$). The input variables for ENVIRO-GRO are λ_1 and ψ . The nitrate production rate is the derivative of eq. (3.6).

The application of organic nitrogen fertilizers is usually associated with tillage events that mix the applied O_N to a specified depth (Pang and Letey, 2000). Specification of such incorporation events using ENVIRO-GRO therefore includes a specification of the amount of organic N (kg ha^{-1}) and the depth of mixing (cm). Conversion of applied organic N (kg ha^{-1}) to a concentration (mmol/g soil) is performed by the program. Details of the data entry are discussed in chapter 4. Incorporation events represent a jump discontinuity in both the concentration of organic N and the rate of conversion to nitrate. In fact, these events reinitialize the organic N concentration profile. Thus, when incorporation events occur, the time step is reduced to the minimum value to accommodate the discontinuity. In summary, the organic N concentration increases when fertilization events occur and decreases slowly due to mineralization which produces nitrate.

Relation of Decay Series to Nitrate Production Rates

The decay of organic materials as a source of plant-available nitrogen (PAN) for crops is commonly represented by decay series (Pratt et al., 1973). These series consist of a sequence of fractions that are multiplied by the potential available N to obtain the amount of N that will be available to the crop each successive year following application. For example, dry corral manure

with a decay series of [0.35 0.15 0.10 0.05] would supply 35% of N applied during the first year, 15% of the remaining amount during the second year, and so on. Note that about one half of the applied N would remain in the organic form after 4 years and clearly would reflect the presence of a slow pool. These series have proved useful for estimating the PAN produced in years following an application and for developing schedules of reduced yearly fertilization amounts that would be needed to meet a crop yield goal. The time periods for N uptake are cropping seasons that are shorter than one year so the yearly decay series data don't provide data of sufficiently short period to be applicable to N uptake while the crop is growing. However, the decay series can be thought of as data points within a continuous decay function as described by eq. (3.6). In general, these data points will not exactly match the proposed function so the parameter values λ_1 and ψ can be estimated by a least-squares process.

The second term in eq. (3.6) represents decay of organic-N contained in the slow pool. This slow decay started when the organic-N material was applied but, initially, the total decay was dominated by the first term representing rapid decay. In order to evaluate ψ the remaining organic-N during the period when slow decay dominates must be extrapolated backwards to the time of application ($t=0$). An example of this procedure was calculated for the decay series [0.4 0.2 0.1 0.05] (Fig. 3).

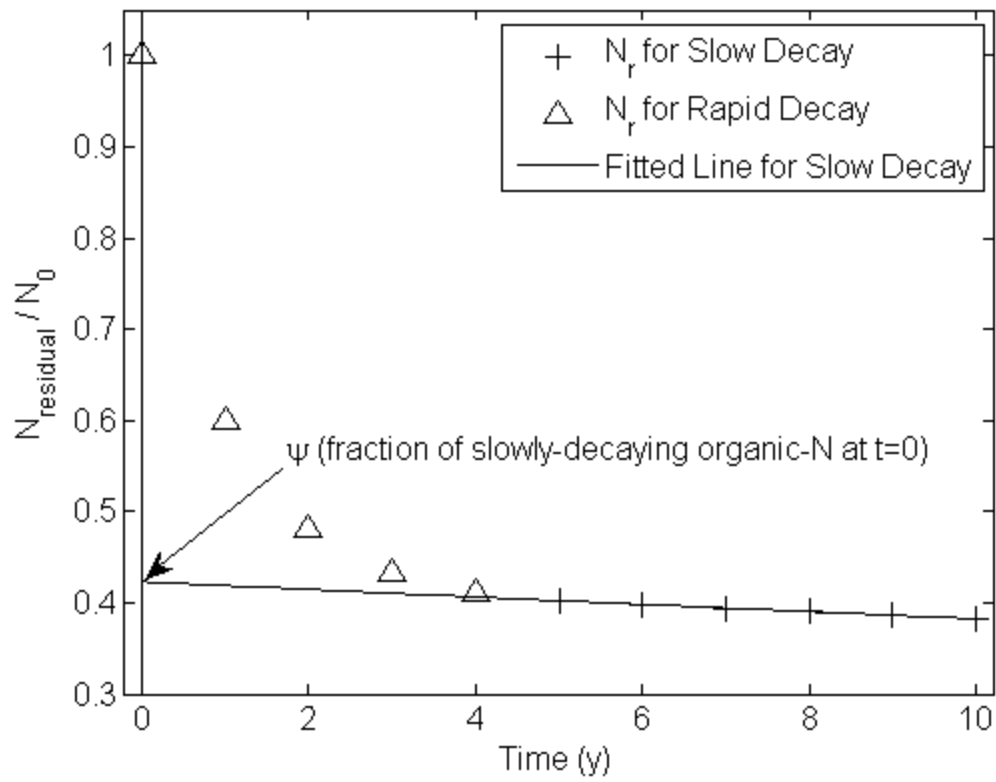
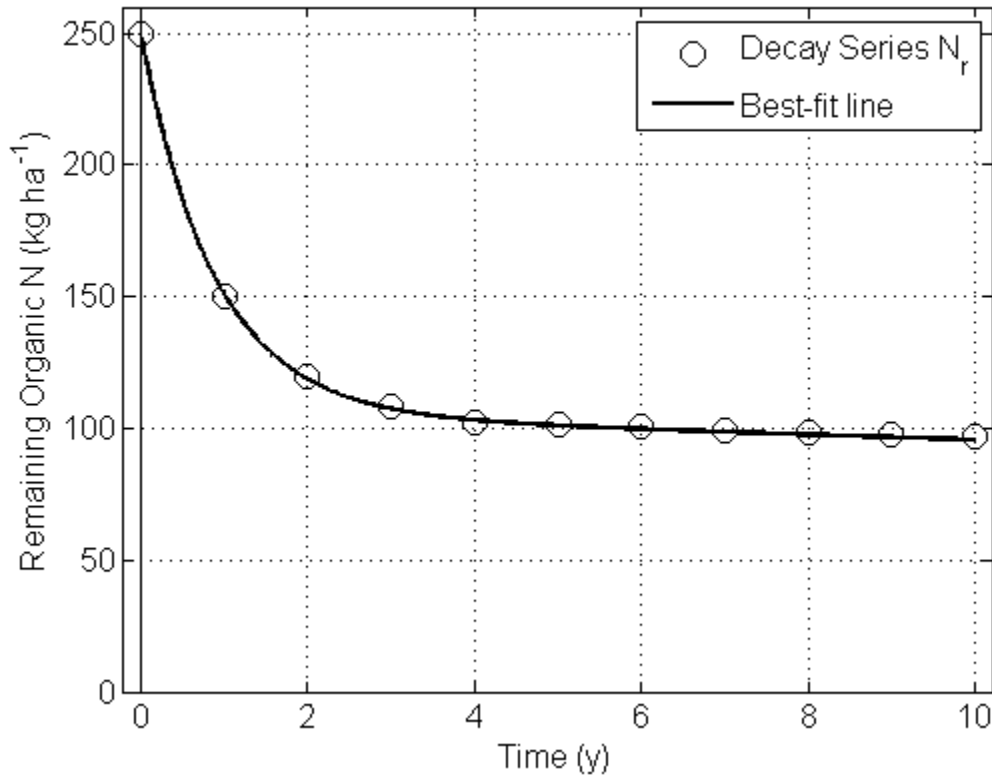


Figure 3, Method for estimating ψ for the decay series [0.4 0.2 0.1 0.05] with a 1% per year decay rate after the fourth year.

When ψ has been determined the remaining parameter, λ_1 , can be obtained by nonlinear least-squares for all the data points (Fig. 3). The values of (ψ, λ_1) for this example are (0.43,



1.134).

Figure 4. Extended decay series [0.4 0.2 0.1 0.05] (circles) and best-fit line.

The ENVIRO-GRO model operates with a time step in units of days but the rapid decay parameter λ_1 has units y^{-1} . In order to use this parameter as an input parameter the units have to be changed to d^{-1} . In doing this the parameter is renamed the N loss rate coefficient:

$$\mu = \lambda_1 / 365.25 \quad (3.7)$$

This parameter value must be supplied in the Basic.in file in order to model decay of organic N. The slow decay process has an N loss rate coefficient of $2.77E-05 d^{-1}$ that is a constant value provided within the program. The N loss rate coefficient corresponding to $\lambda_1 = 1.134 y^{-1}$ is $3.105E-03 d^{-1}$ which corresponds to a half-life for the rapid-decay pool of 223 days.

Application of Inorganic Nitrogen

Inorganic nitrogen is represented exclusively as nitrate by ENVIRO-GRO. Nitrate may be applied at the soil surface by specifying the concentration of NO_3-N in irrigation water. The concentration should be calculated by the user from the amount of N applied ($kg N ha^{-1}$) and the depth of applied irrigation water. For example, consider a $50 kg N ha^{-1}$ application and a 4-cm

depth of irrigation water. The volume of water applied to one hectare is expressed as $depth * (cm^2 / ha) * (L / cm^3)$ or $4 * 1 \times 10^8 * 1 \times 10^{-3}$. The mass of N to be applied is $50 * 1 \times 10^6$ mg. The concentration is $5 \times 10^7 / 4 \times 10^5 = 125 \text{ mg L}^{-1}$. Note, this procedure allows mineral N to be applied during the growing season, but it does not require the N to actually be applied by dissolving it in water. It could be applied at the soil surface and leached into the soil by infiltrating water.

Root Uptake of Nitrogen

Certain attempts at modeling the root uptake of nitrogen and other chemical species have been based on a mechanical conception in which the movement of solutes towards and into a root was the basis of the uptake calculation. This approach has inherent difficulties in the establishment of usable geometries for root systems and the lack of observational detail sufficient to quantify parameter values such as a root permeability coefficient (Pang and Letey, 1998). The ENVIRO-GRO model takes a simpler approach that considers the availability of nitrogen as the significant variable. The model, therefore, presumes a high efficiency of the plant to obtain nitrogen and that N availability is the limiting factor for N uptake.

The N uptake (N_u) by the plant is computed by

$$N_u = N_p(t) \int \beta(z) \alpha_n(z) dz \quad (3.8)$$

Where N_p is the potential N uptake when N is not limiting, $\beta(z)$ is the root density distribution, and α_n is a nitrogen stress factor. A relationship between the N concentration in the soil solution (C_N) and α_n is required. C_N^* is the critical N concentration where α_n equals 1 when C_N is equal to or greater than C_N^* . Pang and Letey (1998) proposed that

$$C_N^* = N_p / T_p \quad (3.9)$$

For weather conditions where T_p is small, such as in the winter time, the value of C_N^* as calculated by this ratio may be unrealistically high and the user may choose a different value based on experimental evidence. ENVIRO-GRO provides for data entry of C_N^* in the boundary condition event file “Bound.In”. The user enters the specific value to be used unless C_N^* is calculated using the ratio. In this case the user enters zero as a placeholder and the program automatically reverts to the calculation based on the ratio (3.9).

If the nitrogen concentration is less than the critical value at any position of the root zone, uptake from that position is less than potential uptake and the integrated uptake is therefore less than potential uptake. There is considerable experimental evidence that if N is deficient in one part of the root zone, that extra N can be taken up from other parts of the root system to compensate. In other words, N would not be deficient for the plant until N was deficient from the entire root zone.

ENVIRO-GRO is programmed to induce extra N uptake from zones where N is excessive to compensate for zones where N is deficient. The initial step computes N uptake without compensation. If N is not deficient in any part of the root zone, the potential N uptake is achieved and no further iteration is required. If N is deficient in all parts of the root zone, computation ceases for that time step. If parts of the root zone has deficient N and other parts have excessive N, the potential N uptake is artificially increased by the amount equal to the original potential uptake minus the computed N uptake. This procedure is iterated until either there is N deficiency throughout the root zone or a maximum of 50 iterations is reached.

The total N uptake for the growing season is computed. The ratio of seasonal actual computed N uptake to seasonal potential N uptake is computed. If the N uptake is proportional to the crop yield, this ratio also represents the ratio of yield to that with no N deficiency. However, if the N uptake and yield are not proportional, the user may wish to make an independent calculation of relative yield from the seasonal values of actual and potential N uptake available in the CropFinal.dat file.

N-deficiency and Water Stress Effects on Potential Water and Potential N Uptake

Under stressed conditions (either water or N or both), the plant canopy is reduced; therefore, the potential transpiration rate should be reduced. Relative plant growth is defined as plant growth relative to growth under unstressed conditions. Relative water uptake is defined as water uptake relative to water uptake without water stress. Relative N uptake is defined as N uptake relative to N uptake when N is not limiting. We assume that the relative plant growth is proportional to the smaller value of the relative transpiration and relative N uptake. The model computes relative water uptake, relative N uptake and the global stress factor (R_f) for each time step. If R_f is less than unity, the effect is a reduction of the plant growth as compared to its potential growth. The smaller size of the plant implies that potential transpiration and potential N uptake are less than would be expected with unstressed conditions. The model presumes that both T_p and N_p are reduced due to the occurrence of deficit conditions in a particular time step. The reduction factor is

$$T_p(t + \Delta t) = T_p(t) + R_f T_p \Delta t / (t - t_{init}) \quad (3.10)$$

where Δt is the length of the time step, t_{init} is the emergence time for the plant and t is the elapsed time during the current growth season. This equation indicates the importance of N-deficiency during early stages of plant growth as compared to later stages when the fractional time factor is much smaller. A similar expression applies to potential N uptake.

Numerical Solution of Water Flow Equation

The Richards equation is nonlinear and requires a numerical solution for the time-varying boundary conditions that are common in agricultural applications. ENVIRO-GRO uses a discretization of the modeled profile that has a user-specified constant nodal spacing. The z-coordinate is positive upwards with the z-coordinate at the base of the profile as a negative number representing the profile depth. The soil surface has a z-coordinate of zero.

Richards Equation

The numerical solution is a mass-lumped finite difference scheme (Simunek et al., 1996; Celia et al., 1990).

$$\frac{\theta_i^{j+1,k+1} - \theta_i^j}{\Delta t} = \frac{1}{\Delta z} \left[K_{i+1/2}^{j+1,k} \frac{h_{i+1}^{j+1,k+1}}{\Delta z} - K_{i-1/2}^{j+1,k} \frac{h_i^{j+1,k+1} - h_{i-1}^{j+1}}{\Delta z} \right] + \frac{K_{i+1/2}^{j+1,k} - K_{i-1/2}^{j+1,k}}{\Delta z} - S_i^j \quad (4.1)$$

The spatial index is i , the temporal index is j and k is index of the current iteration. It is necessary to perform iteration because K , the hydraulic conductivity (cm d^{-1}) is a function of pressure head, h (cm). Δz is the node-spacing and Δt is the time step ($t^{j+1} - t^j$). K at the central points between nodes is given by

$$K_{i+1/2}^{j+1,k} = \frac{K_{i+1}^{j+1,k} + K_i^{j+1,k}}{2} \quad K_{i-1/2}^{j+1,k} = \frac{K_i^{j+1,k} + K_{i-1}^{j+1,k}}{2} \quad (4.2)$$

The sink term S (d^{-1}) is evaluated at the previous time. Eq. (4.1) contains both θ and h in terms that refer to the $(k+1)$ iteration. In order to solve the equation a relationship between the two variables needs to be established for the $(k+1)$ iteration in terms of the k iteration. The term $\theta^{j+1,k+1}$ was expanded in a truncated Taylor series with independent variable h using an expression for the soil water capacity (Celia et al., 1990).

$$C_i^{j+1,k} = \left. \frac{d\theta}{dh} \right|^{j+1,k} \quad (4.3)$$

The left side of (4.1) can then be expressed as:

$$\frac{\theta_i^{j+1,k+1} - \theta_i^j}{\Delta t} = C_i^{j+1,k} \left[\frac{h_i^{j+1,k+1} - h_i^{j+1,k}}{\Delta t} \right] + \frac{\theta_i^{j+1,k} - \theta_i^j}{\Delta t} \quad (4.4)$$

As the iteration proceeds the difference between successive estimates of h_i^{j+1} should diminish to nearly zero making the first term on the right side of (4.4) negligible. Substituting (4.4) and (4.2) into (4.1) yields an equation in tridiagonal matrix form.

$$[P_w]^{j+1,k} \{h\}^{j+1,k+1} = \{F_w\} \quad (4.5)$$

This matrix equation isolates the vector $\{h\}$ so that inversion of the matrix $[P_w]$ followed by multiplication with vector $\{F_w\}$ provides $\{h\}$ for the next iteration. By calculating the maximum absolute value of the difference between successive $\{h\}$, convergence can be established when that maximum value falls below a specified acceptable error. A possible outcome is failure to converge. In that case the program will reduce the time step and perform the entire process again.

Boundary Conditions for Water Flow

Two types of boundary conditions are possible, a Dirichlet condition in which pressure head at the boundary is specified or a Neumann condition of specified water flux (Simunek et al., 1996). For most agricultural problems the boundary condition at the surface will be a Neumann condition that represents either soil surface evaporation when the soil is drying or a specified infiltration rate when an irrigation event is underway. The Dirichlet condition may occur at the surface when water is ponded and the surface pressure head is a positive value indicating the depth of the water.

At the bottom of the modeled profile the boundary conditions may be free drainage or specified pressure head. The free drainage alternative is most often used when the water table is at least 5 m below the bottom of the modeled profile. This boundary condition imposes a water flux at the lower boundary that is equal to the local hydraulic conductivity. Thus, free drainage tends to remove water efficiently from the lower portion of the profile. However, as the water content near the boundary decreases so does the hydraulic conductivity, an effect that tends to limit the overall removal of water from the profile by drainage.

The specified pressure head condition at the bottom of the profile is used to represent water tables that are within about 5 m of the soil surface. By extending the depth of the modeled profile below the water table, the pressure head at the boundary will be a positive value representing the saturated column of water. The specified pressure head condition can either vary with time or be a constant value.

Water Balance Calculation

ENVIRO-GRO has a provision for dividing the modeled soil profile into individual layers. These layers can be used to define the vertical extent of soil units having differing soil properties. Or, they may be used to define a near-surface layer which is mixed during a fertilization event. The soil properties are entered for each soil and that soil is assigned a unique material identification number. This identification number determines which soil is present in a layer. The modeled soil profile thus consists of one or more layers which are further subdivided into elements of equal specified thickness (cm).

Each numbered layer in an ENVIRO-GRO dataset represents a depth range. If no such layers are specifically defined then the entire modeled profile makes up a single layer. The user may also

define different materials within the modeled profile which may or may not correspond to the numbered layers. However, each different material must have at least one layer defined for it. The water balance and chemical balance calculations apply to individual layers.

The mass balance error for water is:

$$M_e = \int_{t_1}^{t_2} q_{in} dt - \int_{t_1}^{t_2} q_{out} dt + \int_L \theta(z, t_2) dz - \int_L \theta(z, t_1) dz - \int_{t_1}^{t_2} \int_L S(z, t) dz dt \quad (4.6)$$

The first two terms represent the volume difference between the cumulative water flux into the layer and the cumulative flux out of the layer between times t_1 and t_2 . The next two terms represent the variation in storage of water for the two times. The depth of water at each time is the integral of the water content over the layer thickness (L). The final term is plant root water uptake which is function of both time and depth so the total depth of water representing uptake over the period between t_1 and t_2 is a double integral.

The numerical procedure for computing the result of (4.6) is

$$M_e = \frac{1}{2} \sum_{i=2}^K (q_{in}(t_{i-1}) + q_{in}(t_i)) \Delta t_i - \frac{1}{2} \sum_{i=2}^K (q_{out}(t_{i-1}) + q_{out}(t_i)) \Delta t_i + \sum_L \theta(t_f) \Delta z - \sum_L \theta(t_s) \Delta z - \sum_{i=2}^K \left[\frac{1}{2} \sum_L (S(z, t_{i-1}) + S(z, t_i)) \Delta z \right] \Delta t_i \quad (4.7)$$

K is the number of time steps occurring between the starting time (t_1) and final time (t_2). q_{in} and q_{out} are the water fluxes at the top and bottom of the layer that are computed at each time step (cm d^{-1}). Δt_i is the i th time step (d) and Δz is the node spacing (cm). The final time is t_f and the initial time is t_i . The variation in storage is obtained by calculating the difference in mass of water present in the layer at these two times. The sink term (d^{-1}) is summed over the thickness of the layer providing an uptake flux for the current time step (cm d^{-1}). These fluxes are summed for all time steps to obtain the total depth of water representing the uptake (cm).

Numerical Solution of the Convection-Dispersion Equation

The convection-dispersion eq. (3.1) is solved by a finite difference approximation of the time derivative on the left side (Simunek et al., 1996). The method is a Crank-Nicholson scheme that is one-half explicit and one-half implicit. This avoids potential instability of a fully explicit formulation in which the concentrations calculated for the current time are exclusively determined from those of the last time step. But the Crank-Nicholson scheme will likely be more efficient than a fully implicit approach.

The spatial discretization is performed using the Galerkin finite element technique (Simunek et al., 1996). A finite series of basis functions represents an approximation of the $c(z, t)$ function in eq. (3.1):

$$c(z, t) \cong \sum_{m=1}^N \varphi_m(z) c_m(t) \quad (4.8)$$

The linear basis functions have a triangular form with the apex located at the nodes and represented using a local variable ζ defined as

$$\zeta = \frac{z - z_{m-1}}{\Delta z} \quad (4.9)$$

Where m refers to a node within the profile and Δz is the nodal spacing. The basis functions are written as:

$$\varphi_{m-1} = 1 - \zeta \quad \varphi_m = \zeta \quad (4.10)$$

At the nodes, the basis functions $\varphi_i(z_j) = \delta_{ij}$ where δ_{ij} is the Kronecker delta defined as unity when $i=j$ and zero for $i \neq j$.

The Galerkin method considers the differential operator to be orthogonal to each of the N basis functions such that:

$$\int_0^L \left[-\frac{\partial(\theta c)}{\partial t} + \frac{\partial}{\partial z} D(\theta, v) \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} v c - S c + S^* \right] \varphi_m dz = 0 \quad (4.11)$$

By substituting $c_m(t)$ for $c(z, t)$ and integrating by parts the resulting equation can be rewritten as

$$\frac{d([Q]\{c\})}{dt} + [S]\{c\} = \{f\} \quad (4.12)$$

Q and S are tridiagonal matrices and $\{c\}$ is the vector of unknown concentrations. These objects are:

$$Q_{nm} = \int_0^L \theta \varphi_m \varphi_n dz \quad (4.13)$$

$$S_{nm} = \int_0^L \left[D(\theta, v) \frac{d\varphi_m}{dz} \frac{d\varphi_n}{dz} - v \frac{d\varphi_n}{dz} \varphi_m - S \varphi_m \varphi_n \right] dz \quad (4.14)$$

$$f_n = \int_0^L S^* \varphi_n dz - q_{sL} \varphi_n(L) + q_{s0} \varphi_n(0) \quad (4.15)$$

q_{s0} and q_{sL} are the material fluxes across the lower and upper boundaries.

The Crank-Nicholson time-stepping scheme has

$$\begin{aligned}
[P]^{j+1} \{c\}^{j+1} &= [Q]^j \{c\}^j + \{F\} \\
[P]^{j+1} &= \frac{[Q]^{j+1}}{\Delta t} + \frac{[S]^{j+1}}{2} \\
[Q]^j &= \frac{[Q]^j}{\Delta t} - \frac{[S]^j}{2} \\
\{F\} &= \left(\{f\}^{j+1} + \{f\}^j \right) / 2
\end{aligned} \tag{4.16}$$

The vector of unknown concentrations $\{c\}^{j+1}$ is obtained by numerical solution of the system (4.16) with accommodation of the boundary elements for either Dirichlet or Neumann boundary conditions (Simunek et al., 1996).

ENVIRO-GRO Input Data Files

The input data for ENVIRO-GRO are contained in ordinary text files that have the suffix “.IN” or “.in”. These files have simple formats to assist the user in preparing them. Comments in the files begin with an asterisk (*) as the first character on a comment line. Multiple comment lines can be inserted sequentially into the files. The subroutines reading the files will skip over all comment lines until a non-comment line is reached. The files can be prepared manually using a text editor or a word processor. All files must be saved in plain text format. For lengthy files it may be worthwhile to prepare the data using a spreadsheet, save it in a text format such as (*.csv) and make subsequent modifications using a text editor. For larger projects involving hundreds or thousands of cases it is advisable to automate the production of the input files using programming languages and tools like perl, awk, sed and the UNIX-style shell scripting languages.

The basic units are length (cm), time (d) and mass (g). Mass units of mg and kg are also used as appropriate. The internal calculations for chemical concentrations use mmol. In the case of salt the program assumes a mixture of CaCl_2 and NaCl with equal charge concentrations for each component. For nitrogen the transportable species is nitrate (NO_3^-) which is represented as mmol N having molecular weight of 14. The organic nitrogen concentration is specified in g/g soil of organic matter and chemical species containing nitrogen such as NH_4^+ . The organic N components are not transportable but concentrations can be changed by mineralization and by fertilization events. A non-reactive tracer species is also included primarily for mass balance testing purposes.

ENVIRO-GRO requires that all individual fields on each line must contain an entry. This is the case even if the entry does not apply to the current simulation. If the number of entries on a particular line does not match the number expected then the program will terminate and an error message will be generated in the ErrLog.dat file.

BASIC.IN File

The Basic.IN file has the following format describing the geometry of a simulation:

*	d	dz	nLayers	NumNP
	200.000000	1.000000	2	201

The variable “d” is the depth of the modeled profile in cm. The height of each element is “dz”. The total number of defined layers is “nLayers” and “NumNP” represents the number of nodes. Nodes are located at the top and bottom of each element so “NumNP” is equal to the number of elements plus one. The example has 200 elements in a depth range of 2 meters.

The next line concerns plant, lower boundary condition and simulation of N transport. The first logical constant indicates whether plant root water uptake and root growth will be simulated. The

second entry is sets the lower boundary to free drainage. If this constant is false the program assumes the lower boundary condition is prescribed matric head. In this case the user must specify the matric head at the lower boundary in the file Bound.IN. If N transport will be calculated the third entry in the line is “True”, otherwise “False”. The fourth entry is nitrogen mineralization rate coefficient (μ in eq. (3.7)). If N transport is not being calculated a zero or some other placeholder number must be entered, do not leave blank. This “hCritA” parameter specifies the lower limit for matric head, in this case -1.0E04 cm.

```
*Plant(T/F) Free Drainage(T/F) Nitrogen(T/F) N-Loss-Rate hCritA
False    True    False    0.000000    -1.000000E+04
```

The next section describes the geometry of the layers:

```
* "LayNum", "MatNum", depths of each layer starting from top layer (cm)
2  1  20.00000
1  2  200.000000
```

The layer identification numbers descend from “NLayers” for the uppermost layer to one for the lowest layer in the profile. The material identification numbers determine, for each layer, which set of soil properties from Soil.in apply to that layer. In this case, the material identification number 1 applies to the top layer which is layer 2.

The mineralization rate of organic N may be reduced from its maximum value for months that have lower average temperature. The user may specify the temperature-dependence of the nitrogen mineralization rate in the final section of Basic.in:

* Organic Nitrogen decay coefficient temperature dependence

```
January    0.25
February   0.25
March      0.50
April      0.50
November   0.50
December   0.25
```

The coefficients are multipliers of μ (Feng et al., 2005). These coefficients may be greater than or less than unity. An entry is required for each month that has a coefficient other than 1.00. The coefficient will default to unity for all other months. If temperature-dependence is not considered then the user should omit the entire section.

TIME.IN File

The first line of the Time.In concerns the specification of output times. For simple cases, the user can specify the output times as uniform which means that a standard interval in days exists between output times. The output times only apply to files that contain substantial amounts of data such as vertical profiles of water content or to water and chemical balance files. Other output files have daily or seasonal values.

```
* Output Times Uniform(0) or Specified(1)
1
* dt0          dtMin          dtMax          dtOut dateInit dateFinal
1.000000E-004 1.000000E-005 1.000000E-001 0.0 6/1/2009 1/15/2015
```

This case has user-specified output times. The initial time step is 1.0E-04. A small initial time step is advisable because the water flow and solute transport may have large fluxes due to the initial conditions. The minimum and maximum time steps are set to 1.0E-05 and 0.1, respectively. The “dtOut” variable represents the interval between print times when uniform output times has been specified. In this case the variable is set to zero. The initial and final dates of a simulation are given in standard U.S. date format (mm/dd/yyyy).

A few lines of the section containing print time specifications are:

```
5
* PrintDate Time(hours,0-24)
06/11/2009 9.00
06/21/2009 9.00
07/01/2009 9.00
```

The times are given in fractional hours so a print time of 9:45 AM would be entered as 9.75. Print times can be entered as required up to a maximum of 1000 entries.

SOIL.IN File

Hydraulic properties of soils are entered in this file following a standard soil water retention and hydraulic conductivity model (van Genuchten, 1980; Mualem, 1976). The five parameters include the volumetric saturated water content (θ_s), the volumetric residual water content (θ_r), the saturated hydraulic conductivity (K_s) and two shape parameters: α and n (2.2). An example of SOIL.IN is:

```
*Number of Soils
2
*MatNum      alpha      Ks      nvq      thR      thS
1            0.039      22.6      1.42      0.050      0.430
2            0.075      106.0      1.89      0.065      0.410
```

The maximum number of soils that can be entered is 20. Each is assigned a material identification number (MatNum). The units for α are (cm^{-1}) and for “Ks” (cm d^{-1}). The other parameters are dimensionless. The values of these parameters can be estimated from easily measureable soil texture and other properties using pedotransfer functions (Carsel and Parrish, 1988; van Genuchten et al., 1991; Schaap et al., 1998). The number of lines of data must correspond to the number of soils entered in the second line of the file. The material identification numbers must start with 1 and increase monotonically to the number of soils that are defined.

PLANT.IN File

This file contains data that are intrinsic to the crop. Those properties that might change depending on planting date or other factors related to the crop schedule are entered in CROPSCHED.IN. An example file is:

```
* Number of Different Crops
1
*ID xRMax  hShres  hPWP  MHThresh  MHSlope
*      cm      cm      cm      dS/m      %/(dS/m)
2    100    -879   -15000    1.7      7.4
```

The maximum number of different crops that can be entered is 20. The crop identification number “ID” must be a positive integer greater than 1. The ID numbers 0 and 1 are reserved for bare soil and a generic grass cover crop, respectively. The maximum rooting depth “xRMax” for each crop is given in cm. The threshold stress for matric head is “hShres”. The matric head causing permanent wilting is termed the permanent wilting point “hPWP”. The h50 value for equation (2.8) is calculated by ENVIRO-GRO as the average of these matric heads. This parameter is the matric head causing a 50% reduction of root water uptake when salinity stress is negligible. The Maas-Hoffman threshold salinity “MHThresh” and the slope “MHSlope” can be obtained from published tables (Maas and Hoffman, 1977). Note that the Maas-Hoffman slope has units of percent reduction per dS/m unit. The program calculates the osmotic head for 50% reduction of root water uptake (π_{50}) and a threshold osmotic head from the Maas-Hoffman parameter values. The threshold osmotic head is the M-H threshold multiplied by two and the slope is the M-H slope divided by two. These conversions take place to account for the Maas-Hoffman data taken as EC_e compared to the plant response to the EC of the soil water as described in chapter 1. The threshold matric and osmotic heads together define a threshold value for the reduction function α_t (2.9).

INIT.IN File

This file provides initialization information that is specific to the layers defined in a simulation. Each layer can have initial values of the concentrations of three transportable species: tracer, salt and NO₃-N. The tracer has units of concentration or mass of solute per liter of solution. The mass unit is defined by the user. Salt is a mixture of NaCl and CaCl₂ in solution in proportions of equal charge. The concentration unit is mg/L in the input file. The molecular weight of the NaCl + CaCl₂ mixture is 56.97 g and ENVIRO-GRO represents concentrations internally as mmol/L. Fixed N is N present as a mineral fertilizer which is incorporated into the soil at the start of a simulation or organic N fertilizer having a complex organic molecular structure. The mineral fertilizer is presumed to dissolve immediately to form transportable NO₃-N. The organic N fertilizer undergoes mineralization of N which gradually releases the transportable NO₃-N species. An example is:

```
* matricHead=1,theta=2 TopValue BottomValue
2    0.250    0.350
*Lay#  Tracer   Salt   FixedN   orgFrac   PsiApp   Mix?
```

*	-	-	mg/L	kg/ha	-	-	(T/F)
2		1.0	227.9	10.0	1.0	0.1	True
1		1.0	227.9	100.0	1.0	0.1	False

The first line of data in this file specifies the initial water content (2) or initial matric head (1). The water content of 0.25 is specified as the volumetric water content that is uppermost in the profile and the bottom of the profile has water content of 0.35. The program will convert water content to matric head and interpolate between the two values to establish the initial matric head profile.

The two comment lines are provided to specify both the constituents and the units required. Entries must be made for all seven data fields. The layer numbers start with the highest number representing the layer at the top of the profile. This conforms to the coordinate system which is positive upward with origin located at the base of the profile. The tracer is a conservative species that has no specified units and is primarily used for testing purposes. Salt concentration is given in units of mg/L as is commonly reported in chemical analyses of water samples. The initial fixed nitrogen consists of organic and mineral components that may have been incorporated in the soil at the start of a simulation. The fraction of organic N has a value between zero and one and the remaining fraction is that of mineral N. The fraction of organic N residing in the slow pool is “PsiApp” meaning the ψ value for the applied organic material. The final entry is Boolean and refers to the capability of a layer or set of layers to be mixed when a fertilization event occurs. The application of organic fertilizer, for example, may occur during tillage which mixes the fertilizer within the top layer of soil. If the Boolean variable is set to “True” then the layer will have existing N concentrations added to the applied N and mixed so that the concentration of N in both organic and mineral form is uniform within the layer.

CHEMIRRIG.IN File

Irrigation water composition is specified in this file. Irrigation waters are assigned identification numbers for specific water compositions. These may be required because the composition of irrigation water may change during a season due to blending. Also, produced groundwater might be substituted for high-quality water delivered through a conveyance system. Fertigation, in which the nitrate content of irrigation water is increased, may also require separately defined water compositions. The calculation of nitrate concentration from applied inorganic N amounts is discussed in chapter 2 (section titled: Application of Inorganic Nitrogen). An example of the file is:

*SolID	TracerTop	SaltTop	NTop	TracerBot	SaltBot	NBot
*	-	-	mg/L	mg/L	-	mg/L
1		1.00	1002.6	0.0	1.0	57.0
						0.0

The maximum number of irrigation compositions that can be defined in this file is 100. Each one must be assigned a unique identification number. Concentration units for salt and nitrate are mg/L and the tracer has arbitrary concentration units.

The user may have access to electrical conductivity of irrigation water rather than chemical composition. A commonly-applied relationship between the electrical conductivity of irrigation water (EC_{iw}) and the total dissolved solids (TDS) concentration (mg/L) is

$$TDS = 640 * EC_{iw} \text{ where } EC_{iw} \text{ is less than or equal to } 5 \text{ dS/m. For } EC_{iw} \text{ greater than } 5 \text{ dS/m:}$$

$$TDS = 800 * EC_{iw} .$$

BOUND.IN File

The schedule of applied boundary conditions is defined in this file. The time of imposition of a new boundary condition is described by the date and fractional hours. The date is written in standard U.S. date format (mm/dd/yyyy). Single digits can be used to specify month and day if that is more convenient. The time of day is specified as fractional hours during the day, for example, 3:45 PM would be 15.75 hours. If an irrigation event lasts six hours and starts at 7:00 AM two records are required to complete the irrigation event. The first record will set the irrigation rate at 7:00 AM and the second record at 1:00 PM would have an entry of zero for irrigation rate. If specific irrigation timing is not required then single daily records can specify the changed values of ETo, “Kc”, N uptake and daily irrigation rate at midnight. The prescribed irrigation flux rate will apply for the following 24-hour period.

A maximum of 4000 records can be entered in the Bound.in file. An example of the file is:

```
* Number of Boundary Conditions
2055
*iBnd Date t(h) ETo Irrig Kc NUptake chmBCTop chmBCBot Sol# C*N hB
1 06/01/2009 0.001 0.726 0.00 0.32 0.000E+000 -1 0 0 0.00 0.0
2 06/02/2009 0.001 0.724 0.00 0.32 7.000E-003 -1 0 0 0.00 0.0
3 06/03/2009 0.001 0.719 0.00 0.32 7.762E-003 -1 0 0 0.00 0.0
4 06/04/2009 0.001 0.706 0.00 0.32 8.607E-003 -1 0 0 0.00 0.0
5 06/05/2009 0.001 0.744 0.00 0.32 9.545E-003 -1 0 0 0.00 0.0
```

This excerpt from the file provides only five records from a file that has 2055. Each record has a sequential ID number, the date and time. The reference crop evapotranspiration rate (“ETo”, cm d^{-1}) is the evapotranspiration rate for a well-watered cool-season grass (Allen et al., 1998). The crop coefficient is a factor that determines the potential daily crop evapotranspiration when multiplied by ETo. The ETo daily values can be estimated by models that vary substantially in complexity and accuracy (Doorenbos and Pruitt, 1977; Hargreaves and Samani, 2003; Allen et al., 1998). Crop coefficients can be determined by weighing lysimeter measurements and are likely to have geographic restrictions due to spatial variation of climate.

The nitrogen uptake can vary over many orders of magnitude so the values are given in exponential format. The unit is $\text{kg ha}^{-1} \text{ d}^{-1}$. The program converts N uptake to $\text{mmol cm}^{-2} \text{ d}^{-1}$ internally. An equation for N uptake for corn was provided by Feng et al. (2005).

The boundary conditions for chemical flux and fixed concentration at the top and bottom of the profile are specified as the same for all three species. A negative value (-1) at the top indicates a prescribed flux which is appropriate for irrigation events having specified water flux. Normally a

negative value would not be specified at the bottom boundary because, in most circumstances, the flux at the bottom boundary cannot be specified. A positive value (1) at the top indicates a fixed concentration boundary condition which would be appropriate in circumstances where a positive pressure head is maintained (ponding). A positive value at the bottom boundary would be used for modeling specified pressure head at the bottom boundary. For example, a positive pressure head at the bottom boundary represents a groundwater table at an elevation above the bottom of the profile. If the model uses the free drainage condition then the bottom boundary condition must be set to zero as shown in the example.

The solution number identifies which solution in ChemIrrig.in will be applied as a result of this change in boundary conditions. If there is no irrigation currently applied (“Irrig” = 0.0) then this identification number can be set to zero. The “ C_N^* ” entry in the file refers to equation (3.9). If this entry is non-zero then the entered value will be substituted for “ C_N^* ” calculated by (3.9).

The final entry is the pressure head (cm) at the lower boundary. In this case the values are all zero because the boundary condition is free drainage. If a shallow water table exists, the profile should be extended below the maximum depth to water that may occur during a simulation. In this situation, the values entered for pressure head will all be positive reflecting the positive pressure exerted by the overlying column of water.

CHEMPAR.IN File

Material parameter values relating to chemical transport are entered in this file. These records are identified by the material identification number. A maximum of 20 different materials can be entered. An example of the file is:

* Mat#	Bulk Density	Dmolecular (cm ² /day)	Dispersivity (cm)
1	1.40	0.026	8.1
2	1.30	0.026	6.2

The first entry is the material ID number. The bulk density (g cm⁻³), molecular diffusivity (cm² d⁻¹) and mechanical dispersivity (cm) are the three data entries. The number of lines in this file must match the number of materials defined in the Soil.in file and the material identification numbers must correspond or an error will be generated.

CROPSCHED.IN File

The crop schedule defines which crops will be entered into a simulation and when they will be grown. The principal data in the file are the planting date, harvest date and an intermediate date when the rooting depth first reaches its maximum value (called RDF Date). Crops are assumed to be planted and harvested on a single day. Individual records can follow each other such that the harvest date of one crop precedes the planting date of the next crop by only a single day. When the program reads consecutive harvest and planting dates like this then there is no fallow period between crops. However, if an interval of one day or more occurs between the harvest date of one crop and the planting date of the next then the intervening period will be assigned either “cropID”=0 or “cropID”=1 automatically. If the question regarding inter-crop periods is answered “True” on the fourth line of the file then the “cropID”=0. Otherwise, the “cropID”=1

corresponding to a grass. An inter-crop period is also defined at the start of a simulation if the simulation begins prior to the planting date of the first crop. The maximum number of records in the file is 30. An example of the file is:

```
* Crop Schedule, number of schedule records is the first line
4
* Are inter-crop periods bare soil? (True/False) (False=cover crop)
True
* CropName CropID PlantDate HarvestDate RDFDate xRMin
  corn      2      6/1/2009  10/15/2009  8/9/2009    2.0
  corn      2     10/16/2009   3/1/2010  12/24/2009   2.0
  corn      2      3/2/2010   7/16/2010  5/10/2010    2.0
  corn      2      7/17/2010  11/30/2010  9/24/2010    2.0
```

The crop name can be up to 20 characters. If it consists of multiple words these should be separated by underscores instead of spaces. The crop name has no function in the program but it is included in some of the output files to improve readability. The “cropID” is a user-specified integer value designating a particular crop. This number must be a positive integer greater than 1 because the ID numbers 0 and 1 are reserved for defining the inter-crop periods. For the example above, all entries refer to the same crop. The planting and harvesting dates can be assigned to any suitable values as long as there is no overlap. The final entry is the minimum rooting depth (cm). The minimum rooting depth should be at least 2 cm in order to avoid numerical problems related to root water uptake from a very limited root zone.

INPUT.IN File

This file contains data regarding fertilization events involving application of organic or mineral fertilizers. Fertilization using irrigation water can be entered using the BOUND.IN and CHEMIRRIG.IN files. An example of the file is:

```
* AtmFall Mineral #_Discrete_Events
0.000000 0.000000 29
* Event# Date AmountApplied orgFrac PsiApp
1 8/01/2009 125.00 1.0000 0.1000
2 10/16/2009 225.00 1.0000 0.1000
3 12/16/2009 125.00 1.0000 0.1000
4 3/2/2010 225.00 1.0000 0.1000
```

The atmospheric deposition of nitrogen is the first entry and the mineral fraction of that deposition follows. However these data are not currently used in the program so enter zeros for them. The number of discrete fertilization events is the last entry. For each event the date is provided and amount in kg/ha. This amount will be mixed among those layers that are so designated in the “Init.in” file. The “orgFrac” entry is the fractional concentration of organic nitrogen contained within the fertilizer. For this example, the fractional concentration indicates that the fertilizer is 100% organic N. The final entry is fraction of the applied organic N that is in the slow pool (eq. (3.6)). Note that these are entered as fractional amounts not percentages.

ENVIRO-GRO Output Files

Overview

Several basic types of output files are generated by ENVIRO-GRO. Files of the profile type contain data that is a snapshot of the entire modeled profile at a specified time. These files have the node number, depth and a set of vectors that represent physical or chemical data within the profile. In order to maintain a manageable size for these data files the profile printouts only occur at times specified in the TIME.IN file. Examples of these data files are CHEMPROF.DAT, STRESSPROF.DAT and WATPROF.DAT.

Single variables representing boundary values, mean values or summed values are printed daily in files that have a time stamp followed by a list of values. These files include DAILYFLUX.DAT, ORGNMASS.DAT, NO3.DAT and REDUC.DAT.

The record of the mass balances for water and the various chemical species are printed at the same specified times as the profiles. The two files are WATBAL.DAT and CHEMBAL.DAT.

The CROPFINAL.DAT file contains data relevant to the end of cropping season. Data include the sum of the root water uptake and the final relative yield. No records are output for fallow conditions unless the fallow crop is entered explicitly in the crop schedule. The ERRLOG.DAT file will only contain entries if errors have been detected. These errors may be generated by incorrect input data file format, numerical problems or file writing issues among others. If a simulation stops unexpectedly this file should be checked because it may contain important debugging information.

DAILYFLUX.DAT

Time (d)	dt (d)	rTop (cm/d)	vTop (cm/d)	vRoot (cm/d)	vBot (cm/d)
153.000	0.11E-01	0.00	0.00	0.23	-0.53
154.000	0.20E-01	0.00	0.00	0.23	-0.53
155.000	0.20E-01	0.00	0.00	0.23	-0.53
156.000	0.20E-01	0.00	0.00	0.23	-0.53
157.000	0.20E-01	0.00	0.00	0.24	-0.53
158.000	0.20E-01	0.00	0.00	0.23	-0.52
159.000	0.17E-01	-1.63	-1.63	0.24	-0.52

The DAILYFLUX.DAT file provides daily mean values for variables related to water flow at the boundaries of the profile. The records are generated at midnight and reflect mean values for the previous day. The mean time step is reported and may be useful in determining whether problems exist in convergence of water flow calculations. If the mean time step is near the minimum time step then convergence problems are likely.

The specified boundary condition for water flow at the soil surface is “rTop”. If soil surface evaporation is specified the values will be positive on days when no irrigation occurred. When irrigation events or precipitation have occurred the value of “rTop” represents the difference between the specified daily soil surface evaporation and the specified irrigation flow. For the example, soil surface evaporation was zero and one irrigation event occurred on day 158. When irrigation events occur the rTop values will normally be negative because irrigation flows will exceed specified soil surface evaporation. The computed flows are “vTop”, “vRoot” and “vBot” (cm d⁻¹), the soil surface water flux, the upward flux of water due to transpiration and the water flux across the bottom boundary, respectively.

NO3.DAT

Time (days)	SumPotNup (kg/ha)	SumActualNup (kg/ha)	Nuptake/PotN (kg/ha/d)	Leach_N (kg/ha)	Tot_Leach_N (kg/ha)	Avail_N (kg/ha)
~						
244.00	0.778E+02	0.145E+02	0.186E+00	-0.821E-03	-0.16695E-02	0.233E+02
245.00	0.780E+02	0.146E+02	0.186E+00	-0.121E-02	-0.28749E-02	0.232E+02
246.00	0.782E+02	0.146E+02	0.187E+00	-0.160E-02	-0.44797E-02	0.231E+02
247.00	0.784E+02	0.147E+02	0.188E+00	-0.218E-02	-0.66624E-02	0.231E+02
248.00	0.785E+02	0.149E+02	0.189E+00	-0.328E-02	-0.99376E-02	0.232E+02

The tilde symbol indicates that some records have been skipped in order to show non-zero values for all of the variables. The NO3.DAT file contains boundary fluxes for NO3-N and a ratio of computed N uptake to potential N uptake. Records are only output for days when fertilization events have not occurred. The potential N uptake is specified in the BOUND.IN input file. If the mass of NO3-N in the current root zone is insufficient to meet the potential uptake rate then N-deficiency occurs and the computed actual N uptake will be less than potential. The leaching of NO3-N from the bottom of the profile is the bottom water flux multiplied by the concentration.

OrgNMass.DAT

Time (d)	OrgN(Top) (kg N/ha)	MinRate (kg N/ha/d)	PANMass (kg N/ha)	OrgN(Next) (kg N/ha)	MinRate (kg N/ha/d)	PANMass (kg N/ha)
153.000	0.200E+03	-0.446E+00	0.425E+00	0.000E+00	0.000E+00	0.168E-01
154.000	0.199E+03	-0.445E+00	0.810E+00	0.000E+00	0.000E+00	0.272E-01
155.000	0.199E+03	-0.444E+00	0.118E+01	0.000E+00	0.000E+00	0.346E-01
156.000	0.198E+03	-0.443E+00	0.154E+01	0.000E+00	0.000E+00	0.395E-01
157.000	0.198E+03	-0.442E+00	0.187E+01	0.000E+00	0.000E+00	0.465E-01
158.000	0.197E+03	-0.441E+00	0.219E+01	0.000E+00	0.000E+00	0.569E-01

The mass of organic nitrogen mass, mineralization rate and PAN mass are given for the two top layers in the profile. The mass of organic nitrogen is calculated as the layer volume multiplied by the N concentration (g/g soil) and the soil bulk density. The mass of nitrogen is increased during fertilization events when organic fertilizer is incorporated into the layer and decreases steadily due to mineralization. The PAN mass varies due to decay of organic fertilizer modified by the effects of transport of nitrate.

CropFinal.DAT

Time (d)	CropID -	Name -	SumRoot (cm)	PotNup (kg/ha)	ActNup (kg/ha)	NProd (kg/ha)	NLeach (kg/ha)	RelYH2O (%)	RelNPotUptake (%)
289.00	2	corn	68.9	300.1	255.6	187.7	46.6	95.5	85.2
426.00	2	corn	62.8	300.1	186.0	234.5	16.3	87.0	62.0
563.00	2	corn	64.8	300.1	206.9	267.8	37.7	89.8	69.0
700.00	2	corn	67.5	300.1	236.9	291.5	36.3	93.5	78.9
837.00	2	corn	69.8	300.1	265.1	308.3	26.4	96.7	88.3

Data compiled at the end of a cropping season are output to this file. The “sumRoot” variable is the depth of water taken up by the crop during the previous season. Seasonal potential N uptake and actual N uptake are “PotNup” and “ActNup”, respectively. “NProd” is the total mass of NO₃-N produced within the modeled profile during the cropping season. “LeachN” is the seasonal total mass of N leached through the boundary at the bottom of the modeled profile. Relative yield, “RelYH2O”, is computed as the ratio of “sumRoot” to the total potential water uptake. “RelNup” is the ratio of total N uptake to total potential N uptake. However, the relative yield computed from N uptake may not be a simple linear function. Therefore the potential and actual N uptake values are included separately providing the user with the data required to define a nonlinear relationship for calculating relative yield that may be more appropriate for a particular crop and growing conditions. An example of a nonlinear function relating the relative N uptake to relative yield for corn is

$$RY = 1.7RN_{up} - 0.7RN_{up}^2 \quad (6.1)$$

where RY is relative yield and RN_{up} is the ratio of actual to potential N uptake (Feng et al., 2005). This particular file demonstrates greater seasonal N uptake during the first season due to the initial NO₃-N content. During later seasons the application of organic nitrogen fertilizer caused increasing N mineralization rates and increasing relative yields.

The CropFinal.dat file is substantially abbreviated when N uptake and transport are not computed. Thus, if the “Nitrogen(T/F)” entry in the Basic.IN file is set to False then the columns for “PotNup”, “ActNup”, “LeachN” and “RelNPotUptake” are omitted from this output file.

WatProf.DAT

Time = 222.38 (d)							
Node	Depth	Mater	h	Theta	K	v	Sink
-	(cm)	-	(cm)	-	(cm/d)	(cm/d)	(1/d)
201	0.00	1	-28.1	0.354	6.00E-01	-9.96E-06	0.000E+00
200	-1.00	1	-27.2	0.356	6.46E-01	-6.36E-02	1.257E-02
199	-2.00	1	-26.3	0.358	6.88E-01	-1.21E-01	1.257E-02
198	-3.00	1	-25.5	0.360	7.27E-01	-1.78E-01	1.257E-02
197	-4.00	1	-24.8	0.362	7.62E-01	-2.35E-01	1.257E-02
196	-5.00	1	-24.1	0.363	7.94E-01	-2.92E-01	1.257E-02

This profile of the variables related to water content and water flow is output every 10 days in this particular simulation. The material identification number is given in the third column.

Pressure head (h) and water content (θ) are the values for the current time step. K is hydraulic

conductivity and v is the water flux. Root water uptake is the final entry and has dimensions of $\text{cm}^3 \text{cm}^{-3} \text{d}^{-1}$.

ChemProf.DAT

Time =	162.29 (d)				
Node	Depth	Tracer	Salt	NO3-N	Org_N
	(cm)	(-/L)	(mg/L)	(mg/L)	(g/g Soil)
200	-1.0	2.8	646.6	312.0	0.122D-03
199	-2.0	2.7	605.9	323.2	0.122D-03
198	-3.0	2.3	525.7	299.0	0.122D-03
197	-4.0	2.0	453.7	273.4	0.122D-03

The ChemProf.DAT file contains concentration data for the three transportable chemical species and the fixed organic N concentration. The data represent the volume element immediately above the node. The concentrations of the transportable species are concentrations within the soil water present so values will increase simply due to a local reduction of water content.

StressProf.DAT

Time =	162.29 (d)				Crop#	1	CropID=	2	corn
Node	Depth	Sink	Alpha	AlphaComp					
-	(cm)	(1/d)	-	-					
201	0.0	0.000E+00	0.00	0.00					
200	-1.0	0.602E-01	0.99	1.00					
199	-2.0	0.602E-01	0.99	1.00					
198	-3.0	0.502E-01	1.00	1.00					
197	-4.0	0.369E-01	1.00	1.00					

This file contains data related to the crop stress and the modification of stress by compensation of root water uptake. The third column is the sink term ($\text{cm}^3 \text{cm}^{-3} \text{d}^{-1}$). The fourth column is the dimensionless reduction function (α) when no compensation occurs. The final column is α after calculating the compensation effect.

WatBal.DAT

Time =	162.38 Days					
Layer#	QCumulBot	QCumulTop	TotUptake	delStore	ABS_ERR	REL_ERR(%)
2	-0.8	-1.64	2.43	-1.66	-0.2E-04	0.0
1	-5.31	-0.87	0.00	-4.44	-0.2E-14	0.0

Water balance is calculated for individual layers in the profile. In this case two layers were defined within a 200-cm profile. The top layer (2) was a plow layer of 20-cm thickness. The output times for water balance are the same as those for the files containing profile data. In this case the balances represent the previous 10 days. The “QCumulBot” and “QCumulTop” are the accumulated mass of water due to water fluxes at the bottom and top of the layer, respectively. The total root water uptake for the layer during the prior 10 days is “TotUptake” (cm). The change in water storage within each layer is “delStore”. “ABS_ERR” represents the absolute value of the error obtained upon summing the contribution and removal of water minus the

change in storage. The relative error is determined by dividing the absolute error by the maximum absolute change in value among the four water masses.

ChemBal.DAT

Time [T]: 212.292

	Tracer	Salt	NO3-N	
Cum. top flux	-0.624E+01	-0.250E+02	0.000E+00	kg/ha
Cum. lower flux	-0.384E+00	-0.154E+01	-0.834E+00	"
Mass in solution	0.937E+02	0.375E+03	0.261E+03	"
Absolute error	0.532E-03	0.213E-02	0.530E-01	"
Relative error[%]	0.001	0.001	0.020	
Mass OrgN (kg/ha)	NO3-N Uptake (kg/ha)	OrgN->NO3-N (kg/ha)		
0.585E+03	0.166E+02	0.147E+02		

The ChemBal.DAT file provides chemical mass balance data for the entire profile. The cumulative top and bottom fluxes provide the change in mass of each species that has occurred over the interval between printouts. The mass in solution is computed from the current concentration profile and the water content. The absolute error is the residual of the sum of the cumulative fluxes and the change in storage. Relative error is the ratio of the absolute error to the mass of the species (%). The mass of organic N that was mineralized during the interval is given under the heading "OrgN->NO3-N".

Examples

Several examples illustrate the use of the ENVIRO-GRO program. These examples are intended to provide simple cases that can be run in order to understand some of the capabilities of the program.

Salt Leaching with No Plants

This example is intended to demonstrate the removal of salt from the soil profile due to leaching. The initial salt concentration is 200 mg/L, uniformly distributed. Irrigation water with zero salt concentration is applied weekly for one day at a rate of 5 cm/day. The potential evapotranspiration is calculated from a 26-year average ETo measured at CIMIS station #2 at the West Side Research and Experimental Center (WSREC) at Five Points, CA. The upward flux of water to the atmosphere is due exclusively to soil surface evaporation. The simulation begins on 6/1/2009 and ends on 10/31/2009.

The input file Basic.in for this example indicates a total depth of 200 cm, node spacing of 1 cm, a single soil layer, and 201 nodes. The Boolean variables indicate no root uptake, free drainage at the bottom of the profile and no consideration of nitrogen. A zero placeholder value is provided for the nitrogen mineralization rate constant and the critical minimum pressure head is set to -1.0E04 cm. The final line in the file specifies a single layer having one soil type and a maximum depth of 200 cm. If two soil types were present then a minimum of two layers would have to be defined.

```
* d      dz      nLayers      NumNP
200.000000      1.000000      1      201
*Plant(T/F) Free Drainage(T/F) Nitrogen(T/F) N-Loss-Rate hCritA
False      True      False      0.000000      -1.000000e+04
1 1 200.000000
```

The input file Bound.in has the first few lines:

```
* Number of Boundary Conditions
153
* iBnd Date t(h) PotETo Irrig Kc NUptake chmBCTop chmBCBot Sol# C*N hB
1 06/01/2009 0.001 0.726 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
2 06/02/2009 0.001 0.724 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
3 06/03/2009 0.001 0.719 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
4 06/04/2009 0.001 0.706 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
5 06/05/2009 0.001 0.744 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
6 06/06/2009 0.001 0.732 0.00 1.00 0.000E+00 -1 0 0 0.00 0.00
7 06/07/2009 0.001 0.739 3.00 1.00 0.000E+00 -1 0 1 0.00 0.00
```

The third entry, “t(h)”, specifies that the boundary conditions will be imposed just after midnight. The potential ETo and irrigation events have units of cm/day. For the case of bare soil evaporation the crop coefficient, “Kc”, normally is assigned the value of 1.0 indicating that the upward flux of water will be equal to potential transpiration when the soil surface is wet. Note the solution number 1 for the irrigation event on June 7 and the rate of application 3 cm/day.

The file specifying initial conditions of the simulation is Init.in:

```
* matricHead=1,theta=2 TopValue BottomValue
2 0.200000 0.350000
*LayerNum Tracer Salt N03-N FixedN orgFrac PsiZero Mix?
* - - mg/L mg/L kg/ha - - (T/F)
1 1.0 200.0 0.0 0.0 0.0 0.0 False
```

The first line specifies that initial values of water content are 0.2 at the top of the profile and 0.35 at the bottom. Because only one layer is present the remainder of the file is just one record indicating a tracer concentration of 1.0 and a salt concentration of 200 mg/L. The remaining data are concerned with nitrogen which is not a subject of this simulation. However, placeholder values must be supplied.

The chemical composition of the irrigation water is specified in ChemIrrig.in:

```
*SolID TracerTop SaltTop NTop TracerBot SaltBot NBot
1 1.0000 0.0000 0.0000 1.0000 0.0000 0.0000
```

The first item is the solution ID number. This is followed by the flux concentrations of tracer, salt and nitrate for the top and bottom of the profile. In this example the flux concentration of the irrigation water is zero.

The computed water content profile starting on DOY 152 (6/1/2009) is:

```
Time = 152.00 (d)
Node Depth Mater h Theta K v Sink
- (cm) - (cm) - (cm/d) (cm/d) (1/d)
201 0.00 1 -227.3 0.200 2.56E-03 6.66E-07 0.000E+00
200 -1.00 1 -226.3 0.201 2.59E-03 -2.85E-05 0.000E+00
199 -2.00 1 -225.3 0.201 2.63E-03 -2.90E-05 0.000E+00
198 -3.00 1 -224.3 0.201 2.67E-03 -2.94E-05 0.000E+00
```

The initial water content at the top of the profile was assigned the value 0.20. The program computed the equivalent pressure head given these data and the soil water retention parameters specified in Soil.in. The sink term is zero at all depths because no root water uptake is occurring.

```
Time = 154.00 (d)
Node Depth Mater h Theta K v Sink
- (cm) - (cm) - (cm/d) (cm/d) (1/d)
```

201	0.00	1	-10000.0	0.081	2.47E-08	8.45E-02	0.000E+00
200	-1.00	1	-1155.6	0.127	1.91E-05	8.12E-02	0.000E+00
199	-2.00	1	-509.5	0.158	2.22E-04	7.20E-02	0.000E+00
198	-3.00	1	-358.6	0.175	6.60E-04	5.93E-02	0.000E+00

The profile two days later has much lower water content in the top few nodes due to soil surface evaporation. The pressure head in the top node has fallen to the minimum boundary pressure that is allowed for the input parameter value (“hCritA” = -1.0E04 cm). The hydraulic conductivity has also decreased by approximately 5 decades for the top node.

Time = 160.00 (d)							
Node	Depth	Mater	h	Theta	K	v	Sink
-	(cm)	-	(cm)	-	(cm/d)	(cm/d)	(1/d)
201	0.00	1	-926.3	0.134	3.71E-05	7.04E-01	0.000E+00
200	-1.00	1	-257.5	0.193	1.74E-03	5.18E-01	0.000E+00
199	-2.00	1	-157.6	0.224	7.23E-03	3.96E-01	0.000E+00
198	-3.00	1	-124.2	0.240	1.43E-02	3.13E-01	0.000E+00

Following the irrigation event at day 158 the water content near the top of the profile increased to approximately 0.3 with a corresponding substantial increase in the matric head. The soil surface evaporation rate has increased due to the greater near-surface water content. The remainder of the simulation follows the same pattern with increasing near-surface water during irrigation events and decreasing water content during the intervening drying periods.

The WatBal.dat file is generated by this simulation because only one layer is present. For multiple layers the program would calculate water balance separately for each layer. A two-day

Time	sumVTop	totInfil	sumVBot	sumSink	Storage	Error
(d)	(cm)	(cm)	(cm)	(cm)	(cm)	(cm)
152.00	0.00	0.00	0.00	0.00	0.00	0.00E+000
154.00	0.25	0.00	-0.49	0.00	-0.74	0.22E-015
156.00	0.11	0.00	-0.30	0.00	-0.41	0.00E+000
158.00	0.08	0.00	-0.23	0.00	-0.31	0.00E+000
160.00	-1.56	-2.26	-0.19	0.00	1.37	-0.22E-015

period was chosen as the output interval “dtOut”. The output times occur at the end of the first time step for each day. The cumulative sums and change in water storage are taken since the last output time. The irrigation event starting at 9:00 AM on day 158 appears in the water balance file on day 160. However, less than 3 cm of cumulative top water flux “sumVTop” is calculated due to ongoing soil surface evaporation. Both the cumulative top water flux and the change in storage are affected by the evaporation. The storage change is also affected by drainage “sumVBot”. The mass balance error is very small for simulations such as this that have no root water uptake.

Solute transport is generally of more interest in agricultural applications than water flow itself. In this simulation the leaching of salt is calculated and the effect can be clearly seen by examining salt concentration in the upper nodes as the simulation progresses (ChemProf.dat).

```
Time = 152.00 (d)
Node   Depth      Tracer      Salt      NO3-N      Org_N
      (cm)      (-/L)      (mg/L)      (mg/L)      (g/g Soil)
  200    -1.0        1.0        200.0        0.0      0.000D+00
  199    -2.0        1.0        200.0        0.0      0.000D+00
  198    -3.0        1.0        200.0        0.0      0.000D+00
```

The initial concentration for the tracer is unity and the salt concentration is 200 mg/L.

```
Time = 160.00 (d)
Node   Depth      Tracer      Salt      NO3-N      Org_N
      (cm)      (-/L)      (mg/L)      (mg/L)      (g/g Soil)
  200    -1.0        2.2        184.0         0.0      0.000E+00
  199    -2.0        1.9        159.5         0.0      0.000E+00
  198    -3.0        1.6        140.4         0.0      0.000E+00
```

Following the first irrigation event on day 158 the salt concentrations near the surface have already fallen dramatically from the initial concentration. The concentration gradient is negative for the top three nodes on day 160 because soil surface evaporation generates increased concentrations as the water content decreases. The tracer concentration has increased because the irrigation water has a tracer concentration of 1.0.

```
Time = 202.00 (d)
Node   Depth      Tracer      Salt      NO3-N      Org_N
      (cm)      (-/L)      (mg/L)      (mg/L)      (g/g Soil)
  200    -1.0        3.9         98.3         0.0      0.000E+00
  199    -2.0        3.5         86.7         0.0      0.000E+00
  198    -3.0        3.1         77.9         0.0      0.000E+00
```

After 40 days of weekly irrigation, the salt concentration in the top three nodes has dropped to less than 100 mg/L but the tracer concentration has continued increasing due to the resupply.

In this example the chemical mass balance is calculated for the entire profile consisting of only one layer. Mass balance is computed as the residual of the sum of chemical fluxes in and out of the profile minus the change in storage. The sign convention is that cumulative top flux is positive because chemical species are entering the profile and cumulative bottom flux is correspondingly negative. The mass in solution is the total mass present in solution within the column.

```
Time [T]: 154.000
-----
---
                        Tracer      Salt      NO3-N
-----
---
Cum. top flux  0.0000E+00 0.0000E+00 0.0000E+00  kg/ha
```

Cum. lower flux	-.6992E+00	-.2455E+01	0.0000E+00	"
Mass in solution	0.6899E+02	0.2422E+03	0.0000E+00	"
Absolute error	0.000E+00	0.000E+00	0.000E+00	"
Relative error[%]	0.000	0.000	0.000	

Time [T]: 264.000

	Tracer	Salt	NO3-N	
Cum. top flux	-.3476E+01	0.0000E+00	0.0000E+00	kg/ha
Cum. lower flux	-.6964E-01	-.2445E+00	0.0000E+00	"
Mass in solution	0.1149E+03	0.2213E+03	0.0000E+00	"
Absolute error	0.862E-03	0.000E+00	0.000E+00	"
Relative error[%]	0.001	0.000	0.000	

The difference in the mass of salt in solution indicates that approximately 21 kg/ha of salt were removed during 100 days of the weekly irrigation treatment. The mass balance errors for each two-day interval were very small for this simulation.

Corn: Multi-season Simulation with Elevated Irrigation Water Salinity

This example is intended to demonstrate the capability of ENVIRO-GRO to perform a multi-season simulation but also to suggest the importance of such simulations when soil salinization may impact crop yield. When irrigation water contains dissolved salts the processes of root water uptake, leaching and continuing application of irrigation water will tend to develop a quasi-steady-state distribution of salinity in the root zone. This occurs because the root water uptake will decrease and leaching will increase as the concentration of salts within the root zone increases.

For this simulation the lower boundary condition for water flow was free drainage and the upper boundary condition was prescribed water flux with irrigation events specified when the water flux (cm d^{-1}) was entered as a positive number. The transfer of water from the soil to the atmosphere was exclusively by transpiration for this example. The crop was corn which had a maximum rooting depth of one meter and a minimum rooting depth of 2 cm at the start of each season. For simplicity, the seasons were back-to-back meaning that the planting date for each successive season occurred on the day after the harvest of the previous crop. The length of each season was 137 days and the same 26-year average ETo from the first example was applied for each crop. Weekly irrigation amounts were structured to match the potential crop evapotranspiration that had occurred during the previous week. The total potential depth of water transpired during the season was 72 cm. The electrical conductivity of irrigation water for this example was 2 dS/m.

The irrigation water chemistry is defined in the file ChemIrrig.in:

```
*SolID TracerTop SaltTop NTop TracerBot SaltBot NBot
* - - mg/L mg/L - mg/L mg/L
1 1.0 1002.6 0.0 1.0 57.0 0.0
```

The SolID parameter is the solution ID number. The salt and NO₃-N concentrations are given in mg/L. The boundary conditions are specified in the Bound.in file:

```
* Number of Boundary Conditions
2055
* iBnd Date t(h) ETo Irrig Kc NUptake chmBCTop chmBCBot Sol# C*N hB
1 06/01/2009 0.001 0.73 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
2 06/02/2009 0.001 0.72 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
3 06/03/2009 0.001 0.72 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
4 06/04/2009 0.001 0.71 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
5 06/05/2009 0.001 0.74 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
6 06/06/2009 0.001 0.73 0.00 0.32 0.000E+000 -1 0 0 0.00 0.00
7 06/07/2009 0.001 0.74 1.63 0.32 0.000E+000 -1 0 1 0.00 0.00
```

Boundary conditions are changed every day at 0.001 h after midnight mainly because ETo and “Kc” are changed daily. Record 7 of the file indicates an irrigation event using irrigation water with “SolID” = 1. The irrigation event spans the 24-hour period starting after midnight so the depth of water specified in the file is the total depth of water applied (1.63 cm). “Kc” is constant for the records shown because the crop is in the early stage of development. The chemical boundary condition at the surface is given the value -1 indicating a flux concentration. At the lower boundary the condition is free drainage so the chemical flux boundary condition must be set to zero. The last two entries in the records are not relevant to this example and are assigned values of zero.

The initial water content was 0.20 at the soil surface and 0.35 at the profile depth of 2 m. The node-spacing was 1 cm. The profile represented a single layer of soil having the soil properties of Panoche clay-loam defined in the Soil.in data file (Oster et al., 2012):

```
* Number of Soils
1
*MatNum alpha Ks nvg thR thS
1 0.039 22.6 1.42 0.050 0.430
```

The van Genuchten shape parameters are “alpha” (cm⁻¹) and “nvg”. The residual and saturated water contents are “thR” and “thS” respectively. The saturated hydraulic conductivity is “Ks” (cm d⁻¹).

The plant parameters provided in the file Plant.in were:

```
* Number of Different Crops
1
*ID xRMax hShres hPWP MHTresh MHSlope
* cm cm cm dS/m %/(dS/m)
2 100 -879 -7121 1.7 7.4
```

The “xRMax” parameter is the maximum rooting depth (cm). The threshold value of matric head for root water uptake is “hShres” (cm). The “hPWP” parameter defines the matric head corresponding to the permanent wilting point. The value listed for “hPWP” was chosen to create a matching h50 to that used in an intermodal comparison study (Oster et al., 2012). A more conventional value would be -1.5E04 cm. The simulations in the comparison study did not include very dry conditions so the differences in terms of results were not expected to be significant. The Maas-Hoffman parameters are the threshold “MHTresh” and the slope “MHSlope”. In this case the Maas-Hoffman threshold is an average EC_e for the root zone of 1.7 dS/m. Relative yield for corn declines with increasing EC_e at a rate of $7.4 \% (dS/m)^{-1}$. These parameter values are used to calculate the threshold for salinity effects on root water uptake and $\pi 50$ (2.8). The computed root water uptake reduction coefficient was $\alpha_{threshold}=0.93$ (2.9). Root water uptake is zero for any value of α computed for nodes in the profile that exceeds the zero intercept.

The schedule of crops is entered using the CropSched.in file. A portion of this file for this example is:

```
* Crop Schedule, number of schedule records is the first line
15
* Are inter-crop periods bare soil? (True/False) (False=cover crop)
True
* CropName CropID PlantDate HarvestDate RDFDate      xRMin
corn        2      6/1/2009   10/15/2009   8/9/2009    2.0
corn        2     10/16/2009   3/1/2010    12/24/2009  2.0
corn        2      3/2/2010    7/16/2010   5/10/2010   2.0
```

The “cropName” parameter must be a continuous sequence of alphanumeric characters with no whitespace so an entry for “dry beans” should contain an underscore or hyphen. The “cropID” can be any positive integer but each different crop must be assigned a different “cropID”. The “RDFDate” is the date when the rooting depth reaches its maximum value. The minimum rooting depth is “xRMin” (cm).

The DailyFlux.dat file provides data for a quick assessment of the validity of the simulation:

Time (d)	dt (d)	rTop (cm/d)	vTop (cm/d)	vRoot (cm/d)	vBot (cm/d)	Evap (cm/d)
153.000	0.20E-01	0.00	0.00	0.23	-0.300	0.001
154.000	0.20E-01	0.00	0.00	0.15	-0.194	0.000
155.000	0.20E-01	0.00	0.00	0.08	-0.159	0.000
156.000	0.20E-01	0.00	0.00	0.09	-0.139	0.000
157.000	0.20E-01	0.00	0.00	0.06	-0.122	0.000
158.000	0.20E-01	0.00	0.00	0.06	-0.108	0.000
159.000	0.12E-01	-1.63	-1.63	0.23	-0.099	0.000

The times shown in this file are just after midnight so the record that is printed represents events that occurred during the previous day. The mean time step was substantially greater than the minimum time step of 1.0E-05 indicating that poor convergence of the water flow computation

was not a problem. The specified irrigation depth for day 158 “rTop” matched the actual infiltrated depth “vTop” indicating that the application rate was sufficiently below the hydraulic conductivity to avoid ponding. The actual transpiration “vRoot” decreased during the early stages of plant growth because the initial water content was 0.20 which generated substantial matric stress and reduced root water uptake. Root water uptake increased to the potential uptake after the wetting of the first irrigation event. Soil surface evaporation was not considered in this simulation so the last column is all zeros except for a small amount on the first day. The free drainage condition was responsible for removal of water from the lower portion of the soil profile which had initial water content near 0.35.

The ChemBal.dat file contains both absolute and relative error for the interval between output times. These mass balance errors are critical for determining whether the other results of the computation are acceptable:

```
Time  [T]:      572.292
-----
---
                        Tracer      Salt      NO3-N
-----
---
Cum. top flux      -.2277E+01  -.4008E+02  0.0000E+00  kg/ha
Cum. lower flux    -.6191E-01  -.2477E+00  0.0000E+00  "
Mass in solution   0.3656E+03  0.5621E+04  0.0000E+00  "
Absolute error     -0.528E-03  -0.929E-02  0.000E+00  "
Relative error[%]      0.000      0.000      0.000
```

The relative error in this case was less than 0.001% indicating that the mass balance calculations confirm the maintenance of high precision for the representation of chemical transport. The cumulative lower flux was substantially smaller than the cumulative top flux indicating salt accumulation in the profile during the 10-day interval. For comparison the record for a much later output time is:

```
Time  [T]:      2132.292
-----
---
                        Tracer      Salt      NO3-N
-----
---
Cum. top flux      -.7698E+01  -.1355E+03  0.0000E+00  kg/ha
Cum. lower flux    -.8920E+01  -.1540E+03  0.0000E+00  "
Mass in solution   0.1030E+04  0.1804E+05  0.0000E+00  "
Absolute error      0.263E-02  0.463E-01  0.000E+00  "
Relative error[%]      0.000      0.000      0.000
```

The cumulative lower flux is greater than the cumulative upper indicating a reduction of the salt mass in the profile during this interval. Other intervals near this output time showed increases in the salt mass suggesting that the salt mass may have reached a steady-state. In fact, a plot of the salt mass in solution demonstrates that salt mass increased slowly after about 12 seasons (Fig. 5).

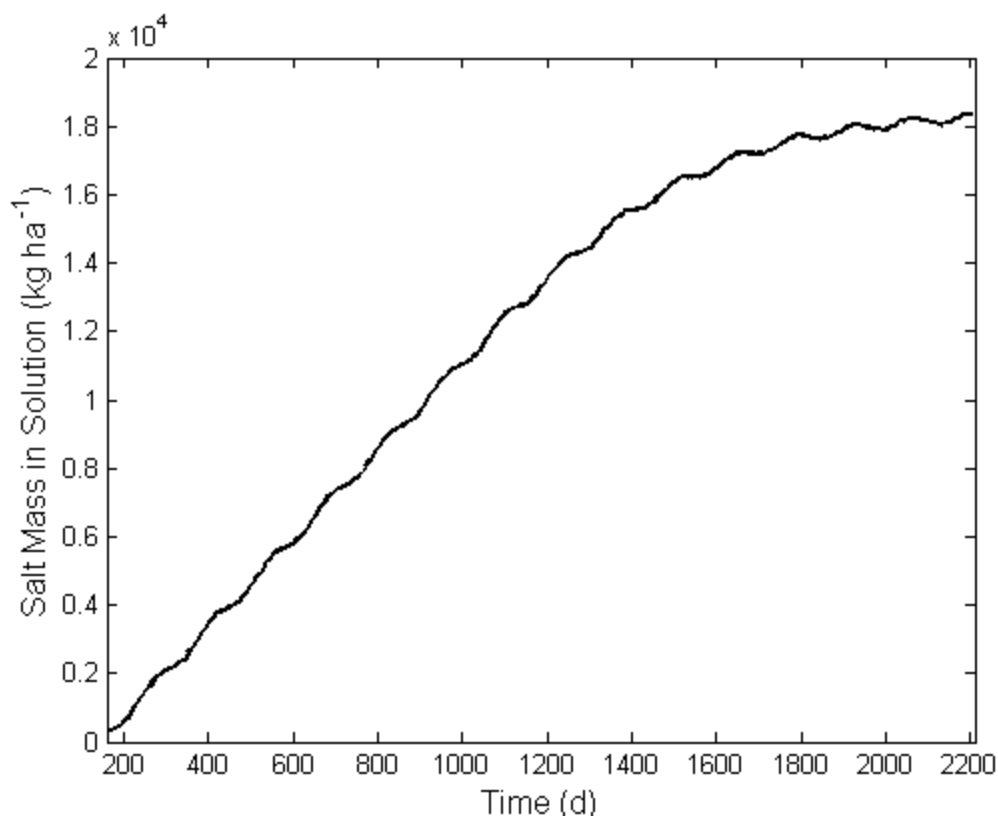


Figure 5. Salt mass in solution taken from ChemBal.dat for irrigation water salinity of 2 dS/m.

Relative crop yield is calculated as the sum of actual transpiration divided by the sum of potential transpiration taken over the entire season. The CropFinal.dat file has relative yield and other variables output at the end of each season.

Time (d)	CropID -	Name -	SumRoot (cm)	RelYH2O (%)
289.00	2	corn	69.3	96.1
426.00	2	corn	72.5	100.0
563.00	2	corn	72.1	99.9
700.00	2	corn	68.7	95.1
837.00	2	corn	68.6	95.0
974.00	2	corn	68.5	94.9
1111.00	2	corn	68.6	95.0
1248.00	2	corn	68.5	94.9
1385.00	2	corn	68.5	94.9
1522.00	2	corn	68.5	94.9
1659.00	2	corn	68.5	94.9
1797.00	2	corn	68.8	95.1
1934.00	2	corn	68.8	95.3
2071.00	2	corn	68.8	95.3
2207.00	2	corn	68.4	95.1

The “sumRoot” variable is the accumulated seasonal root water uptake which is divided by the potential transpiration (~72 cm) to get the relative yield. Relative yield increased for the second

season because initial water content was lower at the start of the first season than at the start of the second. Relative yield decreased after the first three seasons to approximately 95% (Fig. 6).

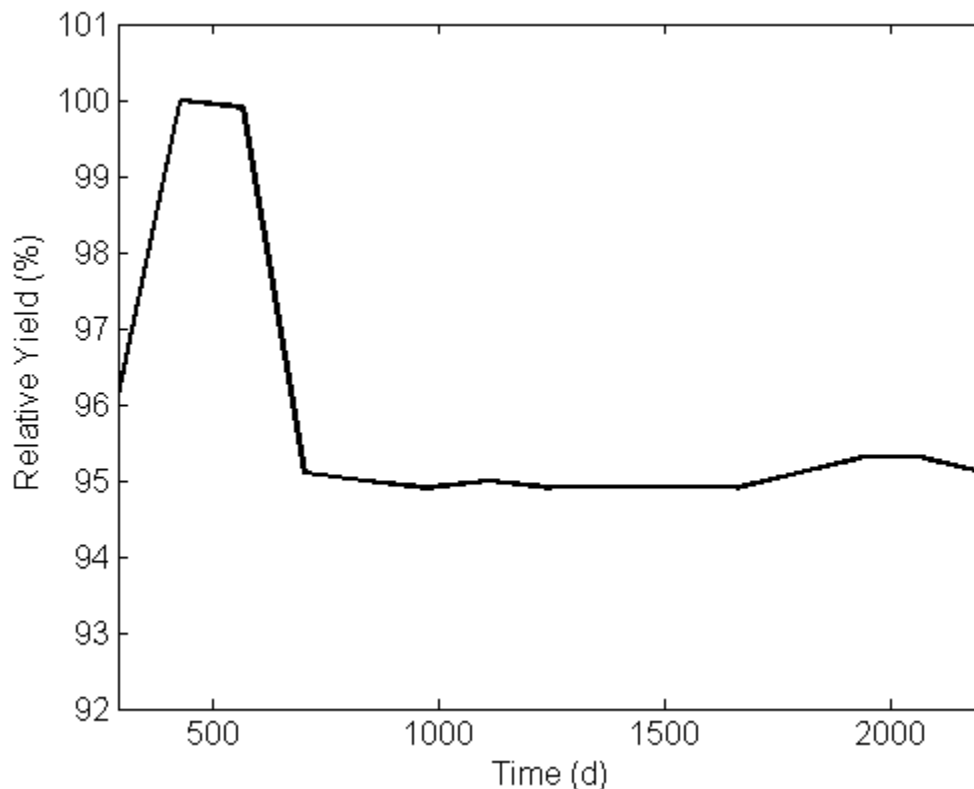


Figure 6. Relative yield vs. time for corn. Data take from CropFinal.dat file.

The relative yield tended to stabilize sooner than the salt mass in solution because root water uptake responded to the salt concentration in the upper 1 m whereas the salt mass represents the entire 2-meter profile. The compensation process tended to amplify this effect because compensation was most effective near the surface due to weekly irrigation.

Corn: Fertilization Using Organic Nitrogen

Reduction of crop yield can occur because of soil salinity issues as in the previous example but can also occur when fertilization is insufficient. ENVIRO-GRO has the capability to represent fertilization by application of inorganic or organic N-fertilizers. These applications are fertilization events in which the fertilizer is mixed into certain prescribed layers in the soil defined by the user. Normally, these mixed layers will be continuous starting from the surface until a depth is reached where no mixing is performed. The combined fertilization and mixing events occur on specified days during either fallow or cropped periods.

Basic.in

The inorganic fertilizers are presumed to dissolve in soil water instantaneously thereby supplying an increased concentration of NO₃-N in the mixed layers. Organic fertilizers are slowly

mineralized producing NO₃-N by a standard decay process. The user needs to specify the decay rate constant “N-Loss-Rate” in the Basic.in file:

```
* d      dz      nLayers      NumNP
200.000000      1.000000      2      201
*Plant(T/F) Free Drainage(T/F) Nitrogen(T/F) N-Loss-Rate hCritA
True      True      True      0.002480      -1.000000e+04
* LayNum, MatNum, depths of each layer starting from top layer
2  1  20.000000
1  1  200.000000
* Organic Nitrogen decay coefficient temperature dependence
January      0.250000
February      0.250000
March      0.500000
April      0.500000
November      0.500000
December      0.250000
```

The Basic.in file contains a Boolean variable indicating that nitrogen transport and uptake will be included in the simulation.

A procedure for obtaining the organic N decay coefficient, λ_1 , was described earlier (Fig. 4).

This coefficient has units of y^{-1} but the time step units for ENVIRO-GRO are days. The nitrogen loss rate is given in grams of NO₃-N per cm² per day so the decay coefficient is divided by 365.25 to obtain the N loss rate coefficient (eq. (3.7)). Often the half-life for the decay process is known rather than the decay coefficient. If this is the case the N loss rate coefficient can be calculated from the half-life using

$$\mu = -\log(0.5) / t_{1/2} \quad (7.1)$$

where $t_{1/2}$ is the half-life (days) and μ is the N loss rate coefficient. The log function is the natural logarithm and the minus sign is needed to obtain a positive value for μ . For the example given above $\mu = 0.00248$ and the half-life would be approximately 280 days.

The example has a near-surface layer of 20 cm depth and a deeper layer extending from 20 cm to 200 cm. The remaining entries in the Basic.in file provide coefficients that define the temperature-dependence of the N loss rate. During the three coldest months of the year the decay coefficient is reduced by a factor of 0.25. These data were included in the file merely to show how they should be entered. The current example doesn't use temperature-dependence because the simulated cropping seasons are back-to-back and don't relate specifically to the calendar.

Init.in

Initial conditions including initial chemical concentrations and water content are defined in the Init.in file:

```
* matricHead=1,theta=2 TopValue BottomValue
2  0.200  0.350
```

*LayerNum	Tracer	Salt	FixedN	orgFrac	PsiApp	Mix?
*	-	mg/L	kg/ha	-	-	(T/F)
2	1.0	227.9	225.0	1.0	0.1	True
1	1.0	227.9	0.0	1.0	0.1	False

The salt concentration in this example is equivalent to an irrigation water salinity of 0.5 dS/m which will have a negligible impact on relative yield. The fixed N concentration is determined from the assumption that 225 kg N/ha is present in the uppermost 20 cm of soil. This 225 kg N/ha represents the amount of N that was applied to the near surface layer at the start of the simulation. The organic fraction of this applied amount is 100%. The ψ value for the applied organic N material is 10% indicating the fraction considered to be in the slow pool (Equation (3.6)). The final entries indicate whether the layer will have fertilizer uniformly mixed into it when fertilization events occur.

Input.in

Fertilizer applications are designated by the Input.in file. An abbreviated set of entries is:

```
* AtmFall Mineral #_Discrete_Events
0.000000 0.000000 29
* Event# Date AmountApplied orgFrac PsiApp
1 8/01/2009 225.00 1.0000 0.1000
2 10/16/2009 125.00 1.0000 0.1000
3 12/16/2009 225.00 1.0000 0.1000
```

The first line contains two variables that are not currently used in the program but are included for potential use in the future. These are atmospheric deposition of nitrogen compounds at the soil surface and the surface application of mineral nitrogen. The number of discrete events is total number of fertilization events that are defined in the remainder of the file. The amount applied N is given in kg/ha that will be divided among all layers defined to be mixing layers. The fraction of organic-N is in the column headed “orgFrac”. The remaining fraction is presumed to be mineral N. In this case all of the applied fertilizer is organic-N. The final entry is the ψ value for the applied organic N (eq. (3.6)).

ChemIrrig.in

Irrigation water chemistry is defined in the ChemIrrig.in file:

```
*Solid TracerTop SaltTop NTop TracerBot SaltBot NBot
1 1.0000 227.8600 0.0000 1.0000 56.9600 0.0000
```

The salt concentration of the irrigation water is 227.86 mg/L or 4 mmol/L which corresponds to an irrigation water EC=0.5 dS/m. The concentrations at the bottom of the profile have no significance because the boundary condition for water flow is free drainage. The irrigation water contains no NO₃-N. If the NO₃-N concentration were greater than zero then inorganic N fertilizer would be added during irrigation events.

Bound.in

The Bound.in file is similar to that of the previous example except that nitrogen uptake is defined:

```
* Number of Boundary Conditions
2055
* iBnd Date t(h) PotETo Irrig Kc NUptake chmBCTop chmBCBot Sol# C*N hB
1 06/01/2009 0.001 0.726 0.00 0.32 0.000e+00 -1 0 0 0.00 0.00
2 06/02/2009 0.001 0.724 0.00 0.32 6.936e-02 -1 0 0 0.00 0.00
3 06/03/2009 0.001 0.719 0.00 0.32 7.688e-02 -1 0 0 0.00 0.00
4 06/04/2009 0.001 0.706 0.00 0.32 8.521e-02 -1 0 0 0.00 0.00
5 06/05/2009 0.001 0.744 0.00 0.32 9.444e-02 -1 0 0 0.00 0.00
6 06/06/2009 0.001 0.732 0.00 0.32 1.047e-01 -1 0 0 0.00 0.00
7 06/07/2009 0.001 0.739 1.63 0.32 1.160e-01 -1 0 1 0.00 0.00
```

The N uptake rate has units of $\text{kg N ha}^{-1} \text{d}^{-1}$. The N uptake rates given in this example would provide a total potential N uptake of 300 kg N per hectare over the entire season (Fig. 7). The

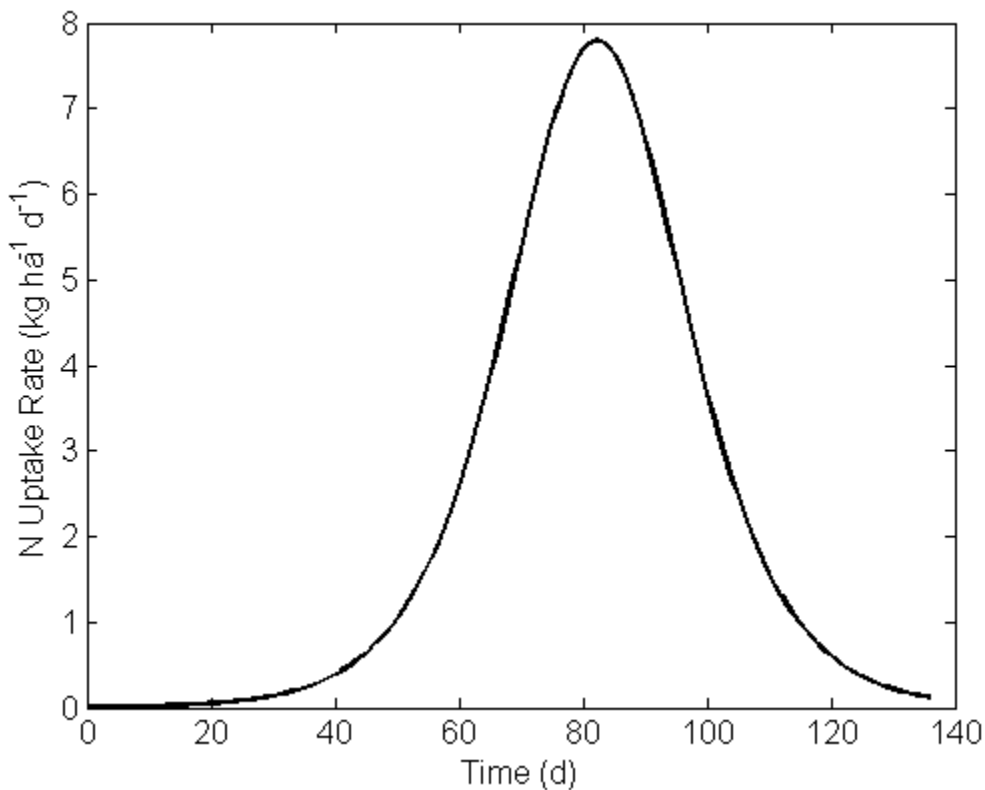


Figure 7. Potential N uptake rate.

remaining input files are very similar to those of the previous example.

OrgNMass.dat

The mineralization rate of organic N is proportional to the amount of organic N present. Negative numbers for mineralization rate indicate the reduction of the organic N concentration due to conversion to NO₃-N. The OrgNMass.dat file contains daily records of the mass of organic N and the mineralization rate for the top two layers in the profile:

Time (d)	OrgN(Top) (kg N/ha)	MinRate (kg N/ha/d)	PANMass (kg N/ha)	OrgN(Next) (kg N/ha)	MinRate (kg N/ha/d)	PANMass (kg N/ha)
153.000	0.224E+03	-0.502E+00	0.478E+00	0.000E+00	0.000E+00	0.189E-01
154.000	0.224E+03	-0.501E+00	0.911E+00	0.000E+00	0.000E+00	0.306E-01
155.000	0.223E+03	-0.500E+00	0.133E+01	0.000E+00	0.000E+00	0.390E-01
157.000	0.223E+03	-0.497E+00	0.213E+01	0.000E+00	0.000E+00	0.523E-01
~						
210.000	0.198E+03	-0.436E+00	0.463E+01	0.000E+00	0.000E+00	0.964E+01
211.000	0.197E+03	-0.435E+00	0.478E+01	0.000E+00	0.000E+00	0.978E+01
212.000	0.197E+03	-0.434E+00	0.495E+01	0.000E+00	0.000E+00	0.989E+01
213.000	0.197E+03	-0.433E+00	0.513E+01	0.000E+00	0.000E+00	0.999E+01
215.000	0.420E+03	-0.932E+00	0.455E+01	0.000E+00	0.000E+00	0.120E+02
216.000	0.419E+03	-0.930E+00	0.453E+01	0.000E+00	0.000E+00	0.128E+02

The initial organic N mass in the top layer was 225 kg N ha⁻¹. The mineralization rate decreases over time until day 214 when the second fertilization event added 125 kg N ha⁻¹. The program does not generate a daily record on days of fertilization events. The second layer was not designated as a mixing layer so the application of organic N was restricted to the top layer. The organic N mass in the top layer increased during the first seven seasons of simulation and subsequently leveled (Fig. 8). Results from this example confirm the idea that multi-season simulations are necessary to fully evaluate the organic N fertilization process (Pang and Letey, 2000).

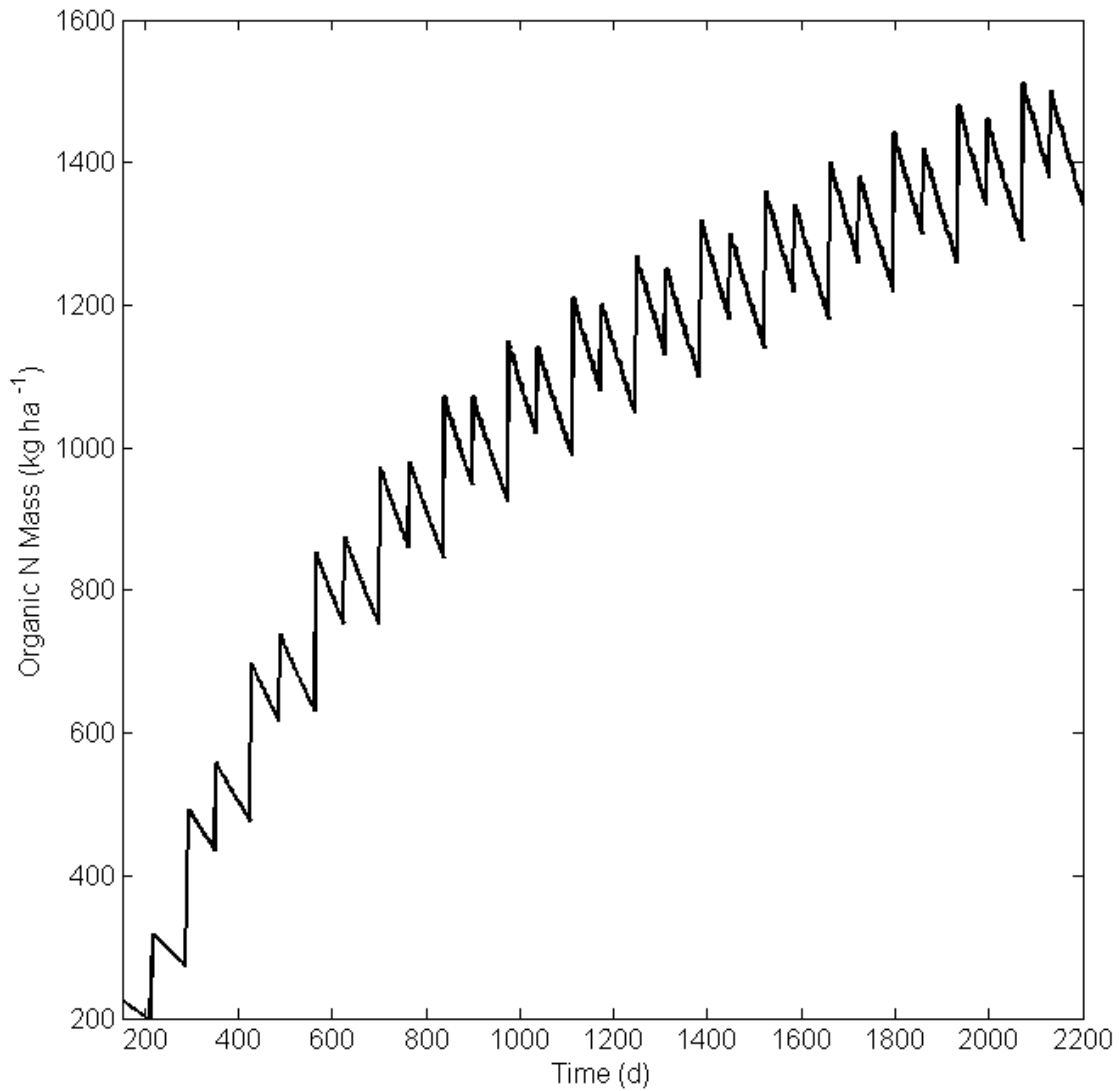


Figure 8. Organic N mass (kg/ha) within the top 20 cm of the soil profile.

NO3.dat

Daily values of cumulative potential and actual N uptake are provided in this file along with the ratio of actual to potential N uptake and daily N leaching rates.

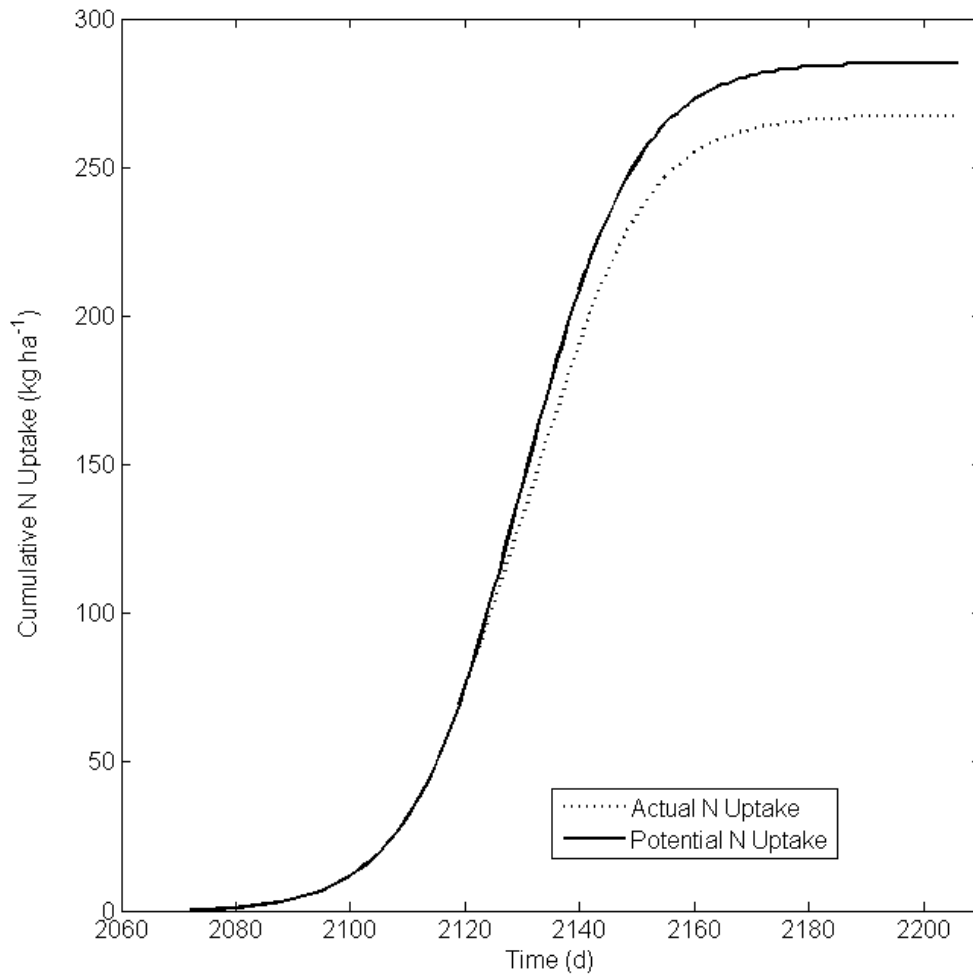


Figure 9. Cumulative potential and actual N uptake for an organic N application rate of 350 kg ha⁻¹.

The cumulative potential N uptake at the end of the first season is approximately 285 kg ha⁻¹ which is less than the prescribed potential N uptake of 300 kg ha⁻¹ (Fig. 9). Thus, the N deficiency caused a reduction of plant growth and consequently smaller potential N uptake (Pang and Letey, 1998). The operation of the reduction factor R_f is described by equation (3.10). The actual N uptake matches the potential until approximately day 2125 when the N uptake rate approaches the maximum. The results indicate that the 125 kg ha⁻¹ application of organic N 60 days after planting was insufficient to meet the subsequent NO₃-N demand.

CropFinal.dat

Crop yield is influenced by salinity, matric stress and nitrogen deficiency. The CropFinal.dat file is substantially expanded when NO₃-N uptake and transport are computed. The table contains entries for actual and potential N uptake, the mass of NO₃-N leached from the bottom of the

profile and the relative calculated as the ratio of actual to potential N uptake. The example file gives results for a seasonal application of 350 kg/ha.

Time (d)	CropID -	Name -	SumRoot (cm)	PotNup (kg/ha)	ActNup (kg/ha)	NProd (kg/ha)	NLeach (kg/ha)	RelYH2O (%)	RelNPotUptake (%)
289.00	2	corn	21.8	300.5	19.7	77.7	2.8	30.2	6.6
426.00	2	corn	36.1	300.5	60.8	146.1	26.1	50.0	20.2
563.00	2	corn	44.7	300.5	101.0	195.0	42.0	61.9	33.6
700.00	2	corn	50.4	300.5	134.3	229.5	48.9	69.9	44.7
837.00	2	corn	54.6	300.5	161.3	254.4	51.6	75.7	53.7
974.00	2	corn	57.9	300.5	183.9	272.4	52.5	80.2	61.2
1111.00	2	corn	60.4	300.5	202.3	285.0	52.4	83.7	67.3
1248.00	2	corn	62.4	300.5	216.9	294.3	52.1	86.4	72.2
1385.00	2	corn	63.9	300.5	228.5	300.4	50.8	88.5	76.0
1522.00	2	corn	65.2	300.5	238.5	305.1	48.7	90.3	79.3
1659.00	2	corn	66.2	300.5	246.8	308.4	45.8	91.7	82.1
1797.00	2	corn	67.4	300.5	254.1	313.0	42.6	93.1	84.5
1934.00	2	corn	67.7	300.5	258.7	312.5	40.4	93.9	86.1
2071.00	2	corn	68.3	300.5	263.3	314.0	39.2	94.6	87.6
2207.00	2	corn	68.4	300.5	267.2	312.4	37.1	95.1	88.9

The relative yield based on water uptake computed from actual transpiration is greater than relative yield computed from the nitrogen uptake ratio “RelNPotUptake”. Note that the potential and actual N uptake values are provided so that the user can calculate relative yield from some other formula than simply the ratio “ActNup”/”PotNup”. During the first season the relative N uptake was greatly reduced by the small initial organic N concentration (225 kg/ha). Relative N uptake increased in the second and subsequent seasons as plant available N increased within the soil profile. Applying Liebig’s Law of the Minimum, the predicted relative yield would be that obtained using actual and potential N uptake rather than that obtained from water uptake. Leaching of N increased during the first six seasons but then decreased as the N uptake process became more efficient.

Three different treatments involving varying application rates of organic N were simulated and the results demonstrate the points made above regarding accumulation of organic N leading to increased mineralization rates and increased relative crop yield over time (Fig. 10)

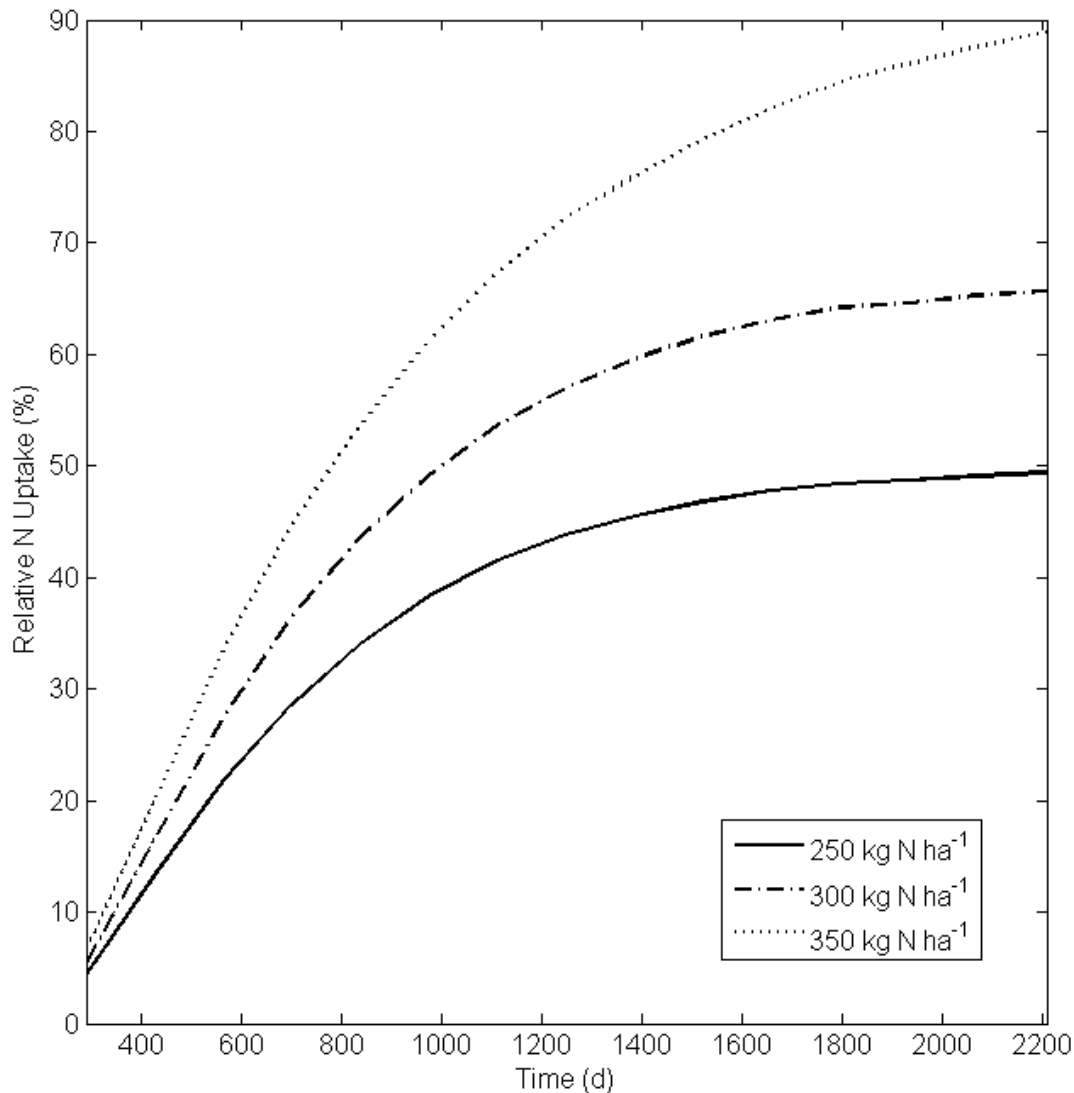


Figure 10. Relative N uptake is the ratio of actual to potential N uptake for three levels of organic N application per season. Data values are plotted for times corresponding to the end of each of 15 seasons.

The relative N uptake is computed as actual N uptake divided by potential N uptake. The N application rate of 350 kg N ha⁻¹ season⁻¹ produced a final relative N uptake of 89% after 15 seasons. Depending on the relative yield model applied, the relative yield calculated from N uptake may be less than the relative yield computed using root water uptake which was 95%. One factor causing this loss of efficiency was the removal of N by leaching. If relative yield were simply calculated as the ratio of actual N uptake to maximum potential N uptake (300 kg/ha) then the final relative yield would be 89% as given in the final entry in the “RelNPotUptake” column of the CropFinal.dat table. This computed value is close to the relative yield calculated

by subtracting the cumulative leached N from the total N produced and dividing by the total applied N $((312-37)/300) = 0.92$. This result indicates that the simulation is approaching a steady-state condition as can be seen in the graph (Fig. 10).

ENVIRO-GRO Installation and Operation

The executable program file is named “EnviroGro.exe”. This file can be placed in any folder provided that folder is accessible to the user. The “DataPath.txt” file should be placed in the project folder containing the input data files. This text file contains the file path to the project folder. For example, a valid “DataPath.txt” file will contain a single line such as:

```
C:\users\myname\documents\projects\OrgNSimulation
```

The “OrgNSimulation” project folder would contain the input files for that particular simulation. In order to run the program a command prompt window, available in the Windows Accessories, can be opened. The “cd” command can be used to change folders to the project folder. The Enviro-Gro program is then executed by entering the complete pathname to “EnviroGro.exe” into the “Command Prompt” window. If the “DataPath.txt” and input files are all available the program should start running and screen output should appear in the command prompt window. When the program completes the simulation the output data files will appear in the project folder.

If the program fails to start properly then it is likely that a formatting error occurred in one of the input files. Check the “ErrLog.dat” file to get information about the error.

Automating ENVIRO-GRO Operation

Often many simulations are required to obtain a complete picture of the plant response to varying inputs such as irrigation, fertilization and stress effects. Considerable redundancy of operations exists in carrying out a program of simulations by just running each separately. These kinds of operations can be easily automated using a UNIX-type shell language. Such UNIX-type emulators are available for Windows as either freeware or commercial products. An example of a Bourne-shell script to execute ENVIRO-GRO in all subfolders below the project folder level is:

```
#!/bin/sh
count=1
for dirname in `ls`
do
  if [ -d "$dirname" ]; then
    echo "$dirname"
    cd "$dirname"
    C:/Users/myname/Documents/Work/exec/EnvGro2012
    cd ..
    count=`expr $count + 1`
    echo "$count"
  fi
done
```

The first line is a comment line that also designates the following script to be interpreted by the Bourne shell. Directory names of all the subfolders are obtained by the “ls” command and are stored as a vector. Each element of the vector is then processed separately in the “do” loop. The “if” test separates ordinary files in the folder from the subfolder names and only processes the subfolders. The “cd” command changes the current folder to the subfolder and the command to execute the ENVIRO-GRO is given as full path starting with the C:\ root folder. It’s sometimes useful to get some output from these scripts while they’re running so two “echo” commands give the current folder and a count of the number of simulations that have been run.

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