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## VARIABLY SATURATED 2-DIMENSIONAL NITROGEN TRANSPORT

by

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#### SUMMARY:

A model for estimating variably saturated 2-dimensional nitrogen transport developed from the United States Geological Survey's VS2DT computer model is presented. Calculated results are compared to observations from a field study performed at Plymouth, NC. To illustrate the potential usefulness of the model a hypothetical example is given comparing nitrogen behavior under two different water management and fertility treatments.

#### KEYWORDS:

Nitrogen, Nitrate, Leaching, Soil, Groundwater

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#### INTRODUCTION

For many years computer models have been used to predict soil nitrogen movement and transformations for agricultural Use of these models are often limited to specific conditions associated with a type of cultural practice or soil. The complete nitrogen cycle is very complex, so researchers have typically considered only the major N reactions, e.g., nitrification, mineralization, immobilization, denitrification, and ammonium adsorption. Furthermore, virtually all nitrogen models have assumed one-dimensional, vertical flow/transport, because of the tendency to consider agricultural fields to be horizontally uniform. A recent issue of Fertilizer Research devoted to soil N modeling in agriculture is a case in point. the fourteen models reported, all were one-dimensional The one-dimensional assumption may not be (Dewilligen, 1991). appropriate under conditions where the moisture content with depth or nitrogen loading at the surface is known to vary in the horizontal direction.

#### MODEL DESCRIPTION

A model is described herein which accounts for two dimensional, variably saturated nitrogen transport. The model is a modification of the United States Geological Survey's VS2DT computer model (Healy, 1990). VS2DT stands for variably saturated, 2-dimensional transport. Since VS2DT was developed for single-solute transport it was necessary to modify the model to handle a multi-solute situation. The modified version of VS2DT will here be referred to as VS2DNT and account for reactive nitrogen transport.

To illustrate the problem we will consider a tile drained field (Fig. 1). At the upper surface of the modelled cross-section is a growing crop. On the right hand boundary of the control area is an optional drainage tile through which water can leave or enter the field system. The left hand boundary is located half-way between drainage tile lines and is an axis of symmetry. Variables which influence the system and which vary on a daily basis include rainfall, potential evapotranspiration (PET), rooting depth, root activity (water and nitrogen uptake), pressure potential in the root, and the total hydraulic head in the drain tile (i.e. water level in the ditch at the field edge).

#### Water Movement

The Richard's equation is used for solving the flow field in time. The flow solution is accomplished using a finite difference numerical technique. The maximum acceptable errors in the total hydraulic head is specified by the user. A time step reduction scheme is used to achieve the desired accuracy. For a detailed description of the flow portion of the model see Lappala, et al. (1987). Values of the water release curve and unsaturated hydraulic conductivity can be entered as input or the

functional relationships developed by Brooks and Corey (1964), Haverkamp et al. (1977) or van Genuchtem (1980) can be used.

During this study the Brooks and Corey (1964) method was used to characterize the relationships between moisture content, pressure head, specific moisture capacity and relative hydraulic conductivity. The Brooks and Corey equations for moisture content,  $\phi$  (cm³/cm³), specific moisture capacity, c<sub>m</sub> (cm¹), and relative hydraulic conductivity, k<sub>r</sub> (dimensionless), as presented by Lappala et al. (1987) are

$$\phi = (\phi' - \phi_r) (h_b/h)^{\check{S}} + \phi_r, h < h_b,$$
 (1)

$$\emptyset = \emptyset', h > h_b, \tag{2}$$

$$c_{m}(h) = -(\emptyset' + \emptyset_{r})(\check{s}/h_{b})(h/h_{b})^{-(\check{s}+1)}, h < h_{b},$$
 (3)

$$c_{m}(h) = 0, h > h_{b},$$
 (4)

$$k_r = (h_b/h)^{(2+3s)}, h < h_b,$$
 (5)

$$k_r = 1.0, h > h_b,$$
 (6)

where, Ø is porosity  $(cm^3/cm^3)$ , h, is the pressure potential (cm),  $h_b$  is the bubbling or air-entry pressure potential (cm), š is a pore size distribution index, and  $\phi_r$  is the residual moisture content  $(cm^3/cm^3)$ .

#### Solute Movement

Solute transport is determined by solving a finite difference form of the advection-dispersion equation. The maximum Peclet Number and Neuman Criteria (Kinzelbach, 1987) are calculated at each time. By controlling the finite difference grid spacing and time step size the Peclet Number and Neuman Criteria, indicators of numerical dispersion and overshoot, respectively, are easily prevented.

Nitrogen pools include solution nitrate, adsorbed nitrate, solution ammonium, adsorbed ammonium, organic-N, and gaseous nitrogen ( $N_2$  and  $N_2$ O). Mineral nitrogen can enter or leave the system with flow from system boundaries. Mineral and/or organic N can be added to the surface directly as in the case of fertilizer. Applying nitrogen to the surface was accomplished by instantaneous addition of the solute to the top row of finite different cells during the first time step of the day of each application. All boundary conditions were allowed to change once in 24 hours during this study, however, it is possible to change boundary conditions at any desired frequency.

Adsorption of nitrate and ammonium can be described by Freundlich or Langmuir isotherms, and ion exchange. During this study, the linear Freundlich relation was used:

 $C'_{a,i} = K_{d,i}C_i(BD/\emptyset)$ , where i is an index (1 ammonium-N, 2 nitrate-N),  $C'_{a,i}$  is the concentration of the solute mass in solid phase (ug/g),  $C_i$  is the concentration of solute in solution expressed in terms of mass per unit mass of dry soil (ug/g),  $K_{d,i}$  is the equilibrium coefficient (cm<sup>3</sup>/g), and BD is soil bulk density (g/cm<sup>3</sup>).

Nitrogen losses or gains from the N pools are incorporated into the advection-dispersion equation as source/sink terms. The source/sink reaction terms were of the form: source/sink =  $C_i k_j$ , where the reaction rate coefficient,  $k_j = k'_j f_j$ , where j is an index (1 nitrification, 2 nitrate-N immobilization, 3 mineralization, 4 ammonium-N immobilization, and 5 denitrification),  $k'_j$  is the reaction rate constant (t¹¹), and  $f_j$  is an function varying between 0 and 1 which may depend on pressure head, moisture content and/or organic-N concentration. The empirical relationships used in this study given below are similar to those used by Hagin and Amberger (1974) except that instead of  $f_2 = f_4 = 1$ , we used  $f_2 = f_4 = f_3$ .

$$f_{1}(h) = 0.2 + 0.005(-h-10) ; -10 cm > h > -10 cm$$

$$0.5 + 0.0015(-h-100) ; -50 cm > h > -100 cm$$

$$1.0 + 0.002(-h-433) ; -100 cm > h > -433 cm$$

$$1 + 0.002(-h-433) ; + 0.00$$

$$f_2(h) = f_3(h) \tag{8}$$

$$f_4(h) = f_3(h) \tag{10}$$

$$f_5 = \frac{\text{orgN}(z)}{\text{orgN}_{\text{max}}} \frac{\phi - 0.8\phi'}{0.1\phi'} ; \quad 0.8 < (\phi/\phi') < 0.9$$

$$\text{orgN}(z)/\text{orgN}_{\text{max}} ; \quad (\phi/\phi') > 0.9$$

$$(11)$$

where orgN(z) is the organic nitrogen concentration which varies with depth, z (cm), and  $orgN_{max}$  is the maximum organic nitrogen concentration (ug/g) in the profile.

In the model the initial organic nitrogen concentration was assumed to decrease exponentially with depth and was estimated by an expression used by Davidson et al. (1979):

$$orgN = orgN_{max}[exp(-0.25z)]$$
 (12)

Crop uptake was described with a Michaelis-Menton type expression similar to that used by Davidson et al. (1979):

$$q_i = C_i(BD/\phi)[q_{max}(t) Q C_i/(K_m + C_i)]$$
 (13)

where  $q_i$  (ug/day) is the root uptake of solute,  $q_{max}$  (dimensionless) is the active solute root uptake factor equal to the ratio of root uptake of solute accounting for diffusion plus mass flow to uptake considering mass flow only , and is a function of time, Q (cm³/day) is the flux of water to the root, and  $K_m$  (ug/g) is the value of  $C_i$  when  $q_i = 0.5q_{max}$ . Because uptake and several of the adsorption processes listed above depend on the concentration (the dependent variable) these processes are nonlinear and are solved by using an iterative procedure.

#### EXPERIMENTAL PROCEDURES

#### Field Site

A study designed to evaluate the model was conducted on a field planted to winter wheat at the North Carolina Tide Water Research Station at Plymouth, North Carolina. Drain tubes (100 mm) were installed 22 m apart on the 13 ha field. The soil, classified as a Portsmouth (Typic Umbraqualt; fine-loamy, siliceous, thermic, 0-2% slope), is typical of the poorly drained soils in the coastal areas of North Carolina. The layout of the drain tiles, the location of the sampling areas and the position of the instrumentation houses (H1, H2, H3) are shown in Fig. 2. The sub-plot (referred to as house 1, 2 or 3) consists of a center tile line and two guard tile lines. The experimental area falls within the area midway between the left guard line and center line and the right guard line and the center line. purpose of the guard lines is to hydraulically isolate the experimental area from adjacent sub-plots.

The study was conducted between February 22, 1991 (Julian date (JD) 52) and June 13, 1991 (JD 163). On February 22, 25 kg/ha potassium-nitrate and 75 kg/ha urea-N was applied to the field. Through May 1 (JD 121) the field water management system was maintained in a free drainage mode. Except where noted below, the water was managed in a controlled drainage mode after May 1.

#### Field and Laboratory Measurements

Measurements were made of outflow rates during drainage from the drain tubes and continuously sampled for water quality. Proportional samples, which were obtained during each drainage event, flowed directly into containers stored inside continuously recorded throughout the study. For a detailed description of the field site and the data acquisition system see Munster et al. (1990).

A weather station at the site measured temperature, rainfall, solar radiation, wind speed and direction, and relative humidity on a continuous basis. Sensors were connected to a Campbell Data Logger and stored on a cassette tape. On several dates, when data were lost due to instrument problems, the data record was supplemented from data collected from the Research Station instrument approximately 3 km from the site. PET values used as input to the model were calculated using the Jensen-Hayes method which is based on solar radiation, temperature, and vapor pressure.

Soil samples were collected for moisture content, nitrate-N and total ammonium-N analysis on a weekly basis. These samples, collected at 15 cm increments to a depth of 90 cm, were composites of three individual samples taken from the sampling areas shown in Fig. 2. Since many sample holes would result over the sampling period which could cause groundwater contamination, all sample holes were filled immediately with soil taken from the edge of the field. All soil samples were immediately frozen at the site, returned to the NCSU Soil Science Department in a cooler, and stored at 4°C until analyzed.

Groundwater was sampled using nested monitoring wells (see Fig. 3). Wells consisted of 5 cm diameter PVC pipe with 15 cm long screens (0.0254 cm slot size) at the desired depth. During well installation, a slotted 7.6 cm core barrel was first pushed to a depth of 100 cm to obtain undisturbed samples. The undisturbed soil sample was transported to a nearby instrument house (No. 2) and separated into 10 cm sections. The samples were then dipped into liquid paraffin wax for preservation using the method of Amoozagar (1988).

After obtaining the undisturbed soil core using the 7.6 cm core barrel, a solid stem auger was inserted into the hole and augered to the desired depth (depths ranged from 0.45 m to the impermeable layer at approximately 2.3 m). Disturbed auger cuttings were obtained from the solid stem auger at 10 cm increments and analyzed for percent sand, silt and clay. One bore hole was made to a depth of 6 m for the purpose of obtaining auger cutting samples. Because sand sluffed in from the walls of the auger hole, a jetting device was constructed to remove sand from the auger hole during placement of the well. Where natural sand did not cover the well screen, fine sand was placed around the screen to about 10 cm above and below the screen. Bentonite pellets were then placed above the sand, and a bentonite slurry poured over the pellets to the surface.

Hydraulic conductivities were determined from the undisturbed samples in the lab using a constant head permeameter method. Hydraulic conductivites were determined in-situ using

the time-lag method described by Hvorslev (1951). The field portion of the method involves removing a known volume of water from the piezometer and measuring the rate of water level recovery. The procedure is sometimes referred to as a slug test.

Because the laboratory conductivities were obtained from vertical cores and, because soil water movement during the field slug tests was assumed to be essentially horizontal, it was possible to estimate the hydraulic conductivity anisotropy ratio where the two methods overlapped (30-100 cm). The expression used for the horizontal hydraulic conductivity was:

$$k_h = d^2 \ln[(m L/D) + \{1 + (m L/D)^2\}^{1/2}]/8 L T$$
 (14)

where d is the diameter of the stand pipe (cm), D is the effective screen diameter (cm), L is the length of screen (cm), m is the transformation ratio,  $(k_h/k_v)^{1/2}$ ,  $k_h$  is the horizontal hydraulic conductivity (cm/day),  $k_v$  is the vertical hydraulic conductivity (cm/day), T is the basic time lag (days), equal to 0.37H<sub>o</sub>, H<sub>o</sub>(t) is the normalized water level equal to 1 at instant slug of water remove, 0 at full water level recovery, and t is time (days).

For the analysis, d = 5.08 cm, D = 10.16 cm, L = 30 cm,  $H_o(t)$  was obtained from the field slug test, and  $k_v$  was obtained from the laboratory value if available. If  $k_v$  was not available m was assumed to be 1.

Soil water characteristic curves were determined using porous plates. For the analysis, soil was undisturbed from 0-1000 cm tension, disturbed from 1000 to 15000 cm tension. Bulk densities and porosities were obtained from the undisturbed soil cores.

Soil nitrate and ammonium were extracted using a 1N KCL solution. The extracted solution and groundwater samples were analyzed using the Bactaroid method (Lowe and Hamilton, 1967) for nitrate, and the Hypochlorite procedure for ammonium. Total elemental Nitrogen and Carbon were determined using a Perkin-Elmer PE 2400 CHN Elemental Analyzer.

#### PARAMETER EVALUATION

#### Hydrologic Parameters

Table 1 gives the values of the soil water characteristic curves from 0-30 cm, 30-90 cm and > 90 cm below the surface, respectively, determined from samples taken from the experimental site. The water release curves, except for the -15000 cm were obtained from Muhammad (1991) as the water release data from the paraffined cores did not appear reliable.

Table 2 gives the hydrologic parameters used for the simulation. Values in the table were measured except where noted. Adjustment of parameters was generally limited to parameters not directly measured (e.g. specific storage, bubbling pressure) to achieve agreement between the model and the field observations (i.e, tile outflow and midpoint water table elevation). For example, the model was found to be sensitive to bubbling pressure,  $h_b$ . To improve agreement between the model and the field data, a value of  $h_b = -5.0 \, \text{cm}$  was used for all depths instead of the values of -1.0, -2.0 and -1.0 cm determined from the soil water characteristics for the three depths, respectively.

To use equation 14, the transformation ratio, m, needed to be calculated from  $k_{\text{h}}$  and  $k_{\text{v}}$ . By using the laboratory value for  $k_v$  (30-100 cm),  $k_h$  became the only unknown in equation 14. After a value of kh was determined the hydraulic conductivity anisotropy ratio,  $\ddot{k}'$ , was obtained by taking the ratio of  $k_v$  to It should be noted that the k' value of 1 for 70-100 cm was not assumed but was calculated using an available estimate for  $k_v$ . For 0-30 cm no estimate of  $k_v$  was available, however, since the plow layer extends into these layers and the majority of root growth takes place within these layers, the soil would be fairly well mixed and an assumption of k'=1 is reasonable (Daniels, For depths greater than 100 cm the soils tended to become more sandy with less structure and therefore a k'=1 at depths greater than 100 cm was a reasonable assumption. Prior operation of the drainage system revealed drainage rates that were well below the expected design rates. Efforts were made during the spring of 1990 to clean out the drain lines of roots and sediment, however, relatively little debris was removed and drainage rates did not seem improved. Plugging around the drain tubes was hypothesized, resulting from either physical or chemical conditions, and is currently being investigated. handle this condition in the model,  $K_h$  in the finite difference cells adjacent to the node simulating the drain tube boundary condition was set to 1.5 cm/day.

No field data were available for the specific storage,  $S_s$ . Consequently this parameter was used to improve the fit between the model and the field flow data. Porosities in the table are means estimated from the undisturbed cores.  $h_b$  and  $\check{s}$  were obtained by a trial and error fitting procedure using equation 1 and the soil water characteristic data given in Table 1. The moisture content corresponding to the -15000 cm pressure potential in Table 1 was used for the residual moisture content,  $\varphi_r$ , in Table 2.

A restrictive layer was found to occur at 2.3 m below the surface and extend to at least 4.2 m. The hydraulic conductivity in this layer was found to be 0.8 cm/day from the in-situ slug tests. Figure 4 shows the distribution of sand, silt and clay with depth at the sub-plots. A large increase in silt is evident between 2.3 and 3.25 m below the surface. For purposes of the

simulation the vertical flux through the restrictive layer was assumed to be negligible and the lower boundary of the cross-section was made a no-flow boundary. A ground surface storage resulting from micro-depressions of 1.5 cm was assumed in this study.

#### Transport Parameters

Table 3 gives the transport parameters used in the Plymouth computer simulation. The longitudinal dispersivity  $(\grave{a}_L)$  was used as a fitting parameter but was kept within the range reported by Gelhar et al. (1985) for a 10 m scale of observation. The dimensions of the site cross-section (Fig. 3) were 2.3 m (vertical) by 11 m (horizontal). The transverse dispersivity,  $\grave{a}_I$ , was assumed to be  $(\grave{a}_L/5)$ . Bulk densities (BD) in the Table are means estimated from the undisturbed cores. The initial values chosen for  $k_1-k_5$  were in the range reported by Davidson, et al. (1978). During subsequent runs these parameters were adjusted to improve agreement with the field nitrogen data.

#### Transient Input Variables

Table 4. gives the 110 day record for precipitation (cm), PET (cm), root depth (cm), root activity (cm $^{-2}$ ) at the top (RTTOP) and bottom (RTBOT) of the root zone, pressure head (cm) in the root (HROOT), total hydraulic head within the drain tube (cm) or depth from the land surface to the ditch water level, and solute uptake factor,  $q_{\text{max}}$ , for ammonium-N and nitrate-N, respectively. PET calculated by the Jenson-Hayes method appeared to underestimate PET during days 122-150 and so a value of 1.5 times the calculated PET was used during that period. Root depths were measured in the field and found to be similar to those observed by Skaggs (1978) for Aurora, NC, for wheat.

#### Initial Conditions

Initial nitrogen concentrations are required by the model. Total nitrate-N and total ammonium-N concentrations just prior to the field experiment were not available. Therefore, as a basis for starting the simulation, concentrations measured at the site the subsequent year were used. Minor adjustments were then made (except for the top layer, 0-10 cm) to these values to cause them to better agree with the field data during the first few days of the simulation. Table 5 gives the initial values for total nitrate-N and total ammonium-N concentration with depth.

The initial values of adsorbed and solution solute were calculated from the following relationships:

$$C_{t,i} = (M_i + M_{a,i} + M_{app,i})/(V BD)$$
 (15)

$$C_i = C_{t,i}/(1 + BD k_{d,i}/\emptyset)$$
 (16)

where  $C_t$  (ug/g) is the total solute concentration,  $M_i$  (ug) is the mass of solute in solution,  $M_{a,i}$  (ug) is the mass of adsorbed solute,  $M_{app,i}$  (ug) is the mass of applied solute (e.g., fertilizer), V (cm³) is volume and all other symbols have been previously defined. The above formulae were applied to each finite difference cell in the model each time boundary conditions were changed.

The initial organic nitrogen concentration was determined from equation 12 with  $\operatorname{orgN_{max}}=3000$  ug/g. Figure 5 shows equation 12 compared to the total elemental soil nitrogen concentration with depth for four dates. Because the inorganic forms of nitrogen were relatively negligible compared to the total elemental nitrogen we assume that the total elemental nitrogen concentration was equal to the soil organic nitrogen concentration.

#### RESULTS AND DISCUSSION

In this section a comparison between the VS2DNT simulated results and results from the field study conducted at Plymouth, North Carolina will be presented and discussed. Owing to the large quantity of simulated output most of the comparisons will be presented in graphical form, while the overall mass balance for water, ammonium-N and nitrate-N will be presented in tabular form. The field data shown in the figures are means from houses 1-3, except where noted. After May 1, 1990 (Julian date 121) the calculated means do not include house 3 because it was maintained in a free drainage mode, whereas, houses 1 and 2, like the model, were placed in a controlled drainage mode.

#### Midpoint Water Table Elevation, Cumulative Drainage and Soil Moisture

The midpoint water table elevation and cumulative drainage are shown in Fig. 6. The cumulative drainage is for house 2 only. The midpoint water table elevation was estimated reasonably well by the model. The model tended to raise to the surface more frequently than actually occurred in the field. It should be recognized that the model, for the sake of computational efficiency, spreads the effects of the transient input variables (i.e., rainfall, PET and the total hydraulic head in the drain tube) over the entire day, whereas in reality some of these variables may occur over very short periods of time (e.g. < 1 hr in the case of rainfall). This may account for the overestimation of water table rise during rainfall events where significant runoff may have occurred. Runoff was not measured during this study.

The total simulated infiltration, runoff, drainage volume, evapotranspiration and change in water stored in the profile were

27.7, 12.1, 4.3, 24.6, and 0.9 cm, respectively. The overall water mass balance error was -0.3 cm, an error well within acceptable limits. Table 6 compares the drainage volume for VS2DNT and houses 1 through 3. Except for house 1, the model compares well with the observed drainage volume.

Due to the hydraulic isolation of the sub-plots by the guardlines, lateral seepage was assumed to be negligible but was not verified. Because for most of the study period the three sub-plots were in the same water management treatment (free drainage days 52-121, control drainage days 122-164) there would have been minimal lateral seepage between the three plots. However, at house 1, a drainage ditch ran along the length of the field approximately 40 m south of the south guardline and may have been a cause of lateral seepage (see Table 6, house 1). The subplot north of house 3 was maintained in an identical water management treatment as house 3 so lateral seepage would have been small.

Upward and downward hydraulic gradients were observed within the restrictive layer between 2.3 m 4.2 m below the surface. upward gradients were observed when the water table was low and downward gradients were observed when the water table was high. Figure 7 shows the average hydraulic gradients at the restrictive layer over the study period. The maximum vertical gradient was approximately 0.15 cm/cm (downward) observed on day 150. Assuming a porosity in this layer of 0.35, and a hydraulic conductivity of 0.8 cm/day, the maximum seepage velocity would be 0.34 cm/day (downward) which is of the order of PET. But the average gradient over the study period was only -0.01 cm/cm (upward) and from which the estimated seepage velocity would be 0.03 cm/day (upward). The assumption during the simulation was that the restrictive layer was impermeable and that all vertical flow through it was zero. Along with the possibility of underestimating runoff, this may also help to explain the excessive rise in the simulated water table during wet periods, since there may have been downward seepage during these periods.

Figures 8 and 9 show the soil water content with depth at the midpoint and tile locations. The figures indicate that the simulated moisture content was generally overestimated. Furthermore, the model moisture content seems less sensitive than the field values. This was partially reflected in the fact that the model did not show any real differences between the midpoint and tile locations. The lack of sensitivity of the model can be explained by referring to equation 1, whose independent variable (h) varies between 0 and -15000 cm while the dependent variable,  $\phi$ , only varies between  $\phi_r$  and  $\phi'$  (generally,  $\phi'$  -  $\phi_r$  - 0.3). Consequently, in the case of the top layer, for example, if the midpoint h = -100 and the tile h = -200 cm, the difference in the moisture contents, using equation 1, will only be 0.381 - 0.375 = 0.006 cm<sup>3</sup>/cm<sup>3</sup>, respectively. In general, however, the predicted water contents were in the range of the field values. In the case of Fig. 9, 45-60 cm depth, the fit could have been improved

by using a smaller value for porosity, however, it was not our intention to adjust input data, such as porosity, for which we had relatively high confidence. It should be noted that the only reaction function that depends on the moisture content was denitrification ( $f_5$ , equation 11), where as, functions  $f_1$ - $f_4$  depend directly on h.

#### Soil Nitrogen Concentrations

Figures 10 and 11 give the nitrate-N concentrations with time and depth at the midpoint and tile locations. A rainfall event at the start of the period depressed the predicted nitrate-N concentration in the 0-15 cm layer but rapid conversion of ammonium-N increased the concentration to near the concentration on the day of application. During initial runs of the model it was not possible to regain the nitrate-N concentration in the top layer as the infiltrating water moved significant mass of nitrate-N into the lower layers. The result was an underestimate of concentration in the top layer and an overestimate in the lower layers. It was hypothesized that the observed "hanging up" of nitrate-N observed in the field in the top layer was due either to anion adsorption or by-pass flow through macropores. Thorup and Mehlich (1961) reported an anion exchange capacity of 2.5 me/100g for a Portsmouth soil (A horizon) in Duplin County, Whatever the cause, the effect was analogous to solute By using a value of  $K_{d,2} = 0.55 \text{ cm}^3/\text{g}$  in the 0-10 cm adsorption. layer the desired effect of holding the nitrate-N longer was achieved (Fig. 10).

The observed rise in concentration after day 120 in the 0-30 cm layers was probably due to increased mineralization, perhaps caused by increasing soil temperature, a variable not directly accounted for in the model. A similar increase in concentration was also observed at the 60-90 cm layer after day 120 at the tile location, but no increase was observed between 30-60 cm. The higher concentrations at depth may have resulted from macropore transport through the 30-60 cm layers. This is supported by the fact that prior to day 120 the water table had been falling for over two weeks dropping to more that 1 m below the surface (Fig. 6). The soil may have dried sufficiently to produce cracks and passageways for water and solute to move rapidly to the tile

At depths below 1 m nitrate-N concentrations were very low. At 1.1, 1.3 and 1.7 m below the surface the model and average observed nitrate-N concentrations did not exceed 0.75, 0.4 and 0.15 ug/g, respectively, throughout the study period.

Figures 12 and 13 compare the VS2DNT and observed ammonium-N concentration with depth at the tile and midpoint locations. From the 0-15 cm depth the predicted ammonium-N concentration dropped from 170 ug/g on day 52 to less than 5 ug/g on day 60 and thereafter. VS2DNT did a reasonably good job of estimating the ammonium-N concentration at all depths. At the beginning of the

study the observed concentrations for both ammonium-N and nitrate-N at the 75-90 cm depth at the midpoint location (Fig. 11 and 13) were about double the concentrations observed at the midpoint location and predicted by the model. The elevated concentrations observed at the midpoint location may have been due preferential movement of fertilizer through large pores. The model assumes porous media flow without macropores and, therefore, did not predict a rise in N concentrations in the 75-90 cm depth during the early period of the simulation.

#### Nitrogen Uptake by Plants

Wheat is known to utilize nitrogen in a specific manner during the season. This uptake function (normalized) is shown in Fig. 14 for a winter wheat crop grown in the Coastal Plain region of Virginia (Alley et al., 1990). The simulated, normalized uptake function compares very well to the observed data. order to obtain the simulated curve it was necessary to use the q<sub>max</sub> values given in the figure. It should be noted that even with the large value of 4 for q<sub>mex</sub> from days 45-70, the plant nitrate-N uptake was not enough to lower the predicted nitrate-N concentration in the 0-15 cm layer during that period (Fig. 10). One possible explanation for the drop in concentration in the field is that environmental and/or microbial conditions resulted in an increased rate of nitrate-N immobilization. explanation can not be confirmed, however, what can be stated with some confidence is that the model lacked sensitivity during certain periods; this is probably due to the absence of accounting for certain environmental variables (e.g., temperature, ph, etc.).

The total plant N uptake estimated by the model was 87 The average nitrogen harvested in the grain was 54 kg/ha. Chapman and Carter (1976) reported that for a wheat crop where 59 kg/ha was contained in the grain, 82 kg/ha were found in the grain plus straw; or of the total uptake (grain plus straw) 73% was found in the grain and 27% in the straw. Using this relationship we can estimate the total above ground N uptake for the Plymouth site. The model calculated the total N uptake which included the above and below ground portions. Information on the percent of total N remaining in the roots for wheat was not available, however, Pan et al. (1986) found that between 5% and 15% of the total N remained in corn roots. Assuming 10% of the total N uptake calculated by the model remained in the roots, the total above ground estimate was 79 kg/ha. Table 6 compares the total above ground N predicted by VS2DNT and measured for houses The model did a good job of estimating N uptake. 1 through 3. The table also gives the N use efficiency for VS2DNT and the three treatments.

The simulation indicated that over 95% of N utilized was in the form of nitrate-N. In the simulation this resulted due to the rapid and almost complete conversion of ammonium-N to nitrate-N early in the simulation. The result we obtained for

percent N utilization as nitrate-N is not unreasonable, however, the proportion of a nitrogen species taken into the plant to the total N uptake is not well understood (Jackson, 1991). It is possible that during a unit of time the mineralized nitrogen (as ammonium-N) enters the plant and the nitrate-N thought to be taken up by the plant is lost from the nitrate-N pool in some other way (e.g., immobilization or denitrification).

#### Nitrogen in Drainage Water

The total nitrate-N lost via the drain tile for VS2DNT and houses 1 through 3 are given in Table 6. The model overestimated nitrate-N losses especially in the case of house 3. In general the observed monitoring well nitrate-N concentrations tended to decrease from house 1 to house 3. At house 3, ponding was observed frequently after rainfall events. The low value of tile nitrate-N of 0.6 kg/ha may have been due to the wetter conditions at this subplot which produced more denitrification and lower concentrations. Had the drainage rate at house 1 been similar to houses 2 and 3 the nitrate-N losses to the tileline would probably have been closer to the model value of 3.0 kg/ha. any case, the model estimated the tile nitrate-N loss to within 1.75 kg/ha which is a small absolute error. Figure 15 compares the model estimated nitrate-N concentration of the drainage water with the average observed concentrations. The model tended to over estimate drainage water concentrations.

The simulated nitrate-N lost by the drain tile was calculated by multiplying the non-sorbed nitrate-N concentration at the tile location by the volumetric water flow to the tile. Since the estimated drainage by the model was consistent with that from house 2, the deviation in the estimated nitrate-N tile loss from that observed at house 2 was related to the nitrate-N concentration at the tile line. However, from Fig. 10 it is seen that the model concentrations from 75-90 cm were slightly less than the average observed values. This result may suggest that not all the nitrate at the tile was mobile. Figure 16 compares the nitrate-N concentrations from 30-45 cm and 75-90 cm depths obtained by soil samples and from groundwater sampling wells. The figure indicates very little correlation between the nitrate-N concentrations obtained by the two methods. Smith et al. (1990) found a similar result comparing Bromide concentrations in soil samples with suction lysimeters. At this stage we are unable to explain the reasons for the poor degree of correlation. More research is necessary to better interpret these results.

The total mass of ammonium-N in the drainage water estimated by VS2DNT was 0.8 kg/ha as compared to the average for the three houses of 0.02 kg/ha. The model drastically overestimated in this case. Since the model estimated the soil ammonium concentration near the tile accurately (Fig. 13), and because the model calculates the tile loss by taking the product of the tile flow and solution ammonium-N concentration, the  $K_{\rm d,1}$  value near the tile must be much greater than the value of 3.0 used. It is

very difficult to estimate such low values for tile loss for ammonium-N and nitrate-N. Suffice it to say that the model estimated both of these variables within 1 or 2 kg/ha.

#### Nitrogen Mass Balance

Table 7 gives the VS2DNT estimate for several of the components of the N cycle. The estimated values are not unreasonable for the coastal plain soils of North Carolina. The overall simulation ammonium-N and nitrate-N mass balance errors were 0.16 and 0.54 kg/ha, respectively.

# EXAMPLE OF ESTIMATING WATER MANAGEMENT AND FERTILITY TREATMENT DIFFERENCES

A large portion of coastal watersheds are comprised of poorly drained soils. Agricultural production on these soils requires improved or man made drainage systems which, incidentally, have been used in some locations for over 200 years. Presently there are over two million acres of land utilizing some degree of improved drainage in coastal North Carolina alone.

Previous work (Skaggs and Gilliam, 1981; Gilliam and Skaggs, 1986) has shown that improved subsurface drainage systems can result in a 10-fold increase in the nitrate lost in agricultural drainage water. At the same time phosphorus loss will be decreased by about 10-fold. Nitrate loss to the environment can be greatly reduced by controlling the drainage outlets during certain periods of the year (Gilliam and Skaggs, 1986). The effectiveness of this practice, called controlled drainage, depends on the intensity of management and it may increase phosphorus outflows. Because of the environmental benefits of controlled drainage, it has been accepted as a Best Management Practice (BMP) by regulatory agencies in North Carolina. Structures to achieve control have been cost-shared by the State of North Carolina in nutrient sensitive watersheds for the past six years.

Farmers have also readily accepted controlled drainage because it conserves water and increases yields. Controlled drainage structures have been placed in ditches draining over 175,000 acres in NC. In NC, the acreage coming under controlled drainage is 25,000 to 30,000 acres annually. This practice has also expanded to other areas along the Atlantic Coast with structures being cost shared for water quality purposes in Virginia, Delaware and Maryland. We have been able to predict qualitative effects of the overall practice but have lacked the ability to quantitatively predict the effect of system management. The rapid acceptance of the practice necessitates use of models such as VS2DNT for evaluating specific treatment differences on solute behavior.

As an example of the use of the model four simulations were run using two water management treatments and two fertility treatments. The simulated conditions are shown in Fig. 17. results of several components of the water budget are shown in Table 8. Relative to free drainage, the runoff and tile flow (i.e. drainage volume) for the controlled drainage system changed dramatically. Table 9 give the tile nitrate-N loss, the plant N uptake, denitrification and net mineralization in kg/ha for the free drainage-single N application treatment. The results for the other three treatments are presented as percentages relative to this treatment (i.e., the standard practice). Assuming that it is desirable to maximize plant N uptake and minimize nitrate-N losses in the drainage water, the controlled drainage-split treatment performed the best. For this treatment drainage water nitrate-N was reduced by over 40% and N uptake by the crop was increased by 27% relative to the free drainage-single N application treatment. In both split N application treatments N uptake by the crop was significantly increased.

It is interesting to note that, for the controlled drainage-split N application treatment, denitrification decreased by 9% relative to the free drainage-single treatment. This result is probably due to the fact that even though there were better conditions for denitrification in the controlled drained treatment, the nitrate-N concentrations may have been lower, perhaps due to the large relative increase in N uptake by the crop and/or the timing of the fertilizer applications. This explanation is supported by the fact that the free drainage-split N application treatment also showed a significant reduction in denitrification (11%) and a large increase in plant N uptake (20%). Because dentrification in the controlled drained treatments was relatively low, the relatively lower nitrate-N losses via the drain tile can be attributed to the large reduction in drainage volume (Table 8).

Figure 18 compares the predicted nitrate-N concentration in the drainage water for the four treatments. The free drainage-single treatment rose from 14 mg/L to over 20 mg/L after the 150 kg/ha N application (day 105). The controlled drainage-single treatment increased much less (12 mg/L to 14 mg/L). The two split treatments responded even less due to the low initial application rate (50 kg/ha) on day 105. On day 135 all treatment concentrations increased as a result of a 4.75 cm rainfall after a relatively dry period. Between days 145 and 150 the split treatments responded to the second application of N (100 kg/ha) with their concentrations rising above the respective single N application treatments. After day 152 both split treatments remained above the single treatments for the duration of the simulation.

Figure 19 shows the nitrate-N concentration with depth, at the tile location, for the controlled drainage-single treatment. Relative to the layers near the soil surface, the concentration

at the tile depth (75-90 cm) remained quite low throughout the simulation. However, between days 150 and 200 the tile depth concentration equalled or exceeded those of the upper layers. After day 200, concentrations above the tile depth increased over that of the tile depth. Increased concentrations near the surface resulted from increased mineralization and decreased crop N uptake, while at intermediate depths (45-75 cm) the increased concentrations may have been due to leaching. Figure 20 compares the nitrate-N concentration at the midpoint and tile location 80 cm below the surface (i.e. tile depth) for the control drainagesingle treatment. The figure illustrates the two-dimensional nature of nitrate-N in a tile drained field. The twodimensionality of the nitrate-N distribution can be expected to be even greater in the case of a subirrigation system, if for example, irrigation water is obtained from a deep well having a nitrate-N concentration near zero.

#### MODEL LIMITATIONS

The model possesses several characteristics that may limit its usefulness. The simulations presented above required anywhere from 13 to 16 CPU hours to run on a DEC minicomputer. If other users were making running jobs on the computer system, run-times may have taken as much as 24 hours.

The model does not produce a completely unique solution, that is to say, the model can produce essentially the same results with different combinations of input. This has to do with the fact that some of the physical processes accounted for produce similar effects on the modeled system. For example, an increase in denitrification will produce a decrease in the nitrate-N concentration; but so will an increase in nitrate-N immobilization. In this example both of these processes are controlled by their respective transport parameters ( $k_5$  and  $k_2$ ).

Depending upon the intended use of the simulated results, the quality and quantity of input required may be very expensive. For example, in the case of the validation study presented above a large effort was made to obtain the input data set. However, in the case of the hypothetical simulation example, most of the input data set was obtained from the literature.

Despite the relatively large effort to obtain a good input data set for the validation study, many of the transport parameters used (Table 3) were not available. This represents a significant limitation for using such a model with confidence.

#### SUMMARY AND CONCLUSIONS

A model for estimating variably saturated 2-dimensional nitrogen transport was developed from the USGS VS2DT model. The new model, VS2DNT, in general, performed quite well. However,

both the nitrate-N and ammonium-N lost via the drainage tile were overestimated. On a relative basis the overestimates were large, but on an absolute basis they were small (1-2 kg/ha).

A hypothetical simulation comparing two water management treatments and two fertility treatments for a corn season was presented. The purpose of the hypothetical simulation was to illustrate the potential usefulness of the model for evaluating management practices. The results indicated that by using controlled drainage with a single application of N the total nitrate-N loss to the drain tile was reduce by 46% and that N uptake by the plants was increased 6%, relative to the free drainage system. By using the controlled drainage system but splitting the nitrogen application the drainage water quality benefit was only slightly reduced (46% to 43%) but nitrogen uptake was increase dramatically from 6% to 27%, relative to the free drainage-single N application treatment.

The usefulness of the model may be limited by the large computer time and input data requirement.

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TABLE 1. DRAINAGE BRANCH OF THE SOIL WATER CHARACTERISTIC FOR SOIL SAMPLES OBTAINED AT PLYMOUTH, NC. VALUES GIVEN IN TABLE ARE IN VOLUMETRIC WATER CONTENT.

Depth (cm)	0	-4	-10	-20	-30	-45	-60	- 75	-100	-150	-200	-300	-400	-600	-800	-5000	-15000
0-30	0.470	0.440	0.430	0.420	0.416	0.411	0.407	0.404	0.397	0.388	0.382	0.376	0.366	0.340	0.336	0.172	0.120
30-90	0.350	0.322	0.316	0.309	0.307	0.304	0.303	0.302	0.299	0.295	0.292	0.291	0.285	0.279	0.277	0.136	0.110

>90 0.299 0.274 0.274 0.253 0.247 0.241 0.238 0.235 0.231 0.225 0.221 0.220 0.214 0.210 0.211 0.123 0.100

TABLE 2. HYDROLOGIC PARAMETERS USED IN PLYMOUTH SIMULATION

Depth Below Soil Surface (cm)

	0-10	10-30	30 <b>-</b> 50	50-70	70-100	100-150	150-240
k <sup>'</sup>	1	1	0.1	0.1	1	1	1
k.	7	20	70	180	5	30	375
k <sub>h</sub> S <sub>s</sub> Ø	10 <sup>-9</sup>	10 <sup>-9</sup>	10-6	10-6	10 <sup>-6</sup>	10-6	10-6
ø³.	0.45	0.40	0.33	0.32	0.33	0.31	0.31
$h_b$	<b>-</b> 5	<del>-</del> 5	<del>-</del> 5	-5	<del>-</del> 5	-5	<del>-</del> 5
	0.12	0.12	0.11	0.11	0.11	0.1	0.1
ø <sub>r</sub> Š	0.07	0.07	0.06	0.06	0.06	0.1	0.1

TABLE 3. TRANSPORT PARAMETERS USED IN PLYMOUTH SIMULATION

Depth Below Soil Surface (cm)

	0-10	10-30	30-50	50-70	70-100	100-150	150-240
à <sub>L</sub>	100	150	100	150	50	100	100
àŢ	20	30	20	30	10	20	20
D <sup>'</sup>	10-6	10 <sup>-6</sup>	10 <sup>-6</sup>	10 <sup>-6</sup>	10-6	10-6	10 <sup>-6</sup>
BD	1.1	1.4	1.5	1.5	1.5	1.6	1.6
K <sub>d,1</sub>	0.9	1.7	1.6	0.8	0.7	0.2	0.2
K <sub>d,2</sub>	0.55	0.0	0.0	0.0	0.0	0.0	0.0
k <sub>1</sub> ''	9	3	3	3	3	3	3
k <sub>2</sub>	0.2	0.2	0.2	0.2	0.2	0.2	0.2
k <sub>3</sub>	7x10 <sup>-4</sup>	6x10 <sup>-4</sup>	2x10 <sup>-4</sup>	$2x10^{-4}$	2x10 <sup>-4</sup>	2x10 <sup>-4</sup>	2x10 <sup>-4</sup>
k <sub>4</sub>	0.02	0.07	0.07	0.07	0.10	0.07	0.07
k <sub>5</sub>	0.004	0.03	0.05	0.10	0.30	0.30	0.30
k <sub>m,1</sub>	0.5	0.5	0.5	0.5	0.5	0.5	0.5
k <sub>m,2</sub>	0.5	0.5	0.5	0.5	0.5	0.5	0.5

TABLE 4. INPUT TO VS2DNT WHICH VARIES ON A DAILY BASIS.

JULIAN DATE	PRECIP.	PET	ROOT DEPTH	RTTOP	RTBOT	HROOT	DITCH DEPTH	QMAX NH4	QMAX NO3
55345678901234566789017777777778988888888889999999999012345678901123456789011234567890112345678901123456789011231111111111111111111111111111111111	4200000052000000000000077001000000105050000000000	0.108 0.000 0.151 0.015	991111222333444555555555555555555555555555	๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋๋	0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.0.	-15000 -1	-100 -100 -100 -100 -100 -100 -100 -100		55555555555555555555555555555555555555

TABLE 4. CONTINUED

DATE DATE DEPTH NH4 NO.  125										
126		PRECIP.	PET		RTTOP	RTBOT	HROOT			QMAX NO3
159 0.0 0.52 8 1E-03 1E-03 -15000 -58 0.0 0. 160 0.0 0.55 8 1E-03 1E-03 -15000 -61 0.0 0. 161 0.0 0.58 8 1E-03 1E-03 -15000 -64 0.0 0. 162 0.0 0.48 3 1E-03 1E-03 -15000 -67 0.0 0.	126 127 128 130 131 133 135 136 137 138 140 141 144 144 145 150 155 157 158 159 161	0.00900310010065700000090000000000000000000000000000	0.4228443489999999158995951881443990000000000000000000000000000000000	25 25 25 25 25 25 25 25 25 25 25 25 25 2	33333333333333333333333333333333333333	33.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3.3	-15000 -15000	-5377030000000000111591111136814	1.0000000000000000000000000000000000000	111110000000000000000000000000000000000

# TABLE 5. INITIAL TOTAL NITRATE-N AND AMMONIUM-N WITH DEPTH IN MICROGRAMS PER GRAM

### Depth Below Soil Surface (cm)

<del></del>	0-10	10-30	30-50	50 <del>-</del> 70	70 <b>-</b> 100	100-150	150-240
Ammonium-N	2	2	3	4	3	2	1
Nitrate-N	2	2	_2	2	1	0	0

TABLE 6. VS2DNT SIMULATED RESULTS VS. OBSERVED DATA

	VS2DNT	HOUSE 1	HOUSE 2	HOUSE 3
TIME FLOW (CM)	4.3	2.3	4.1	4.2
TILE NO <sub>3</sub> (KG/HA)	3.0	1.4	1.8	0.6
N UPTAKE (KG/HA)	79.0	62.0	82.0	77.0
N USE EFFIC. (%)	79.0	61.0	81.0	76.0

TABLE 7. VS2DNT SIMULATED COMPONENTS OF N CYCLE FOR PLYMOUTH SITE

	(KG/HA)
DENITRIFICATION	37
NITRIFICATION	204
MINERALIZATION	114
NO <sub>3</sub> IMMOBILIZATION	99
NH <sub>4</sub> IMMOBILIZATION	3
NET MINERALIZATION	12

TABLE 8. PARTIAL WATER BUDGET FROM HYPOTHETICAL SIMULATION

	FREE DRAINAGE (CM)	CONTROL DRAINAGE (CM)	PERCENT CHANGE
INFILTRATION	46.3	40.2	-13%
RUNOFF VOLUME	11.5	17.6	53%
DRAINAGE VOLUME	21.7	13.7	-37%
EVAPOTRANSPIRATION	29.9	31.5	5%

TABLE 9. PARTIAL NITROGEN BUDGET FROM HYPOTHETICAL SIMULATION

	FREE DR SINGLE (KG/HA)	AINAGE SPLIT *******PERCENT	SINGLE	DRAINAGE SPLIT OLUMN 1******
TILE NO3 LOSSES	28	-4%	-46%	-43%
PLANT N UPTAKE	101	20%	6%	27%
DENITRIFICATION	111	-11%	4%	-9%
NET MINERALIZATION	94	11%	-3%	<u>6</u> %

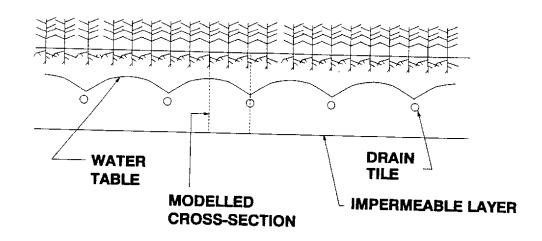


FIG. 1 Modelled cross-section of tile drained field.

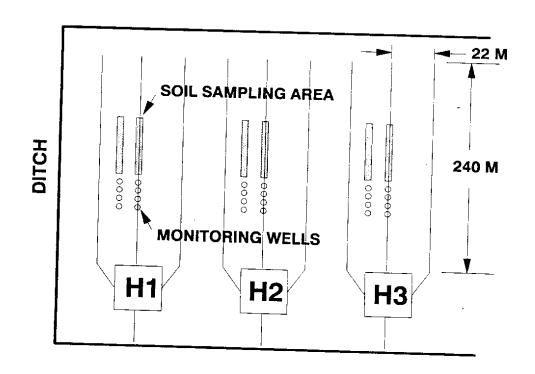


FIG. 2 Plan view of Plymouth study site.

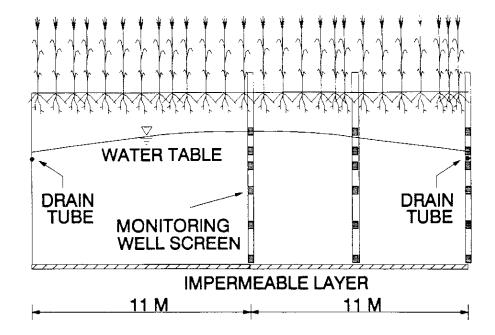


FIG. 3 Vertical cross-section Plymouth experimental site.

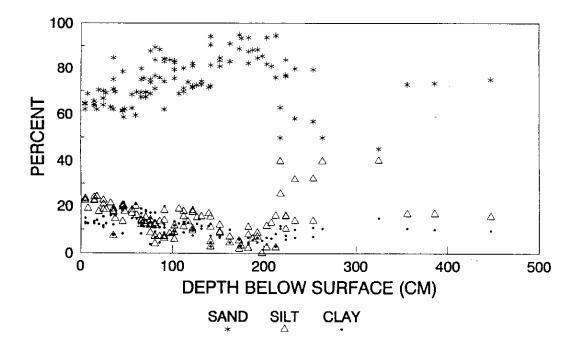


FIG. 4 Percent sand, silt and clay with depth at Plymouth site.

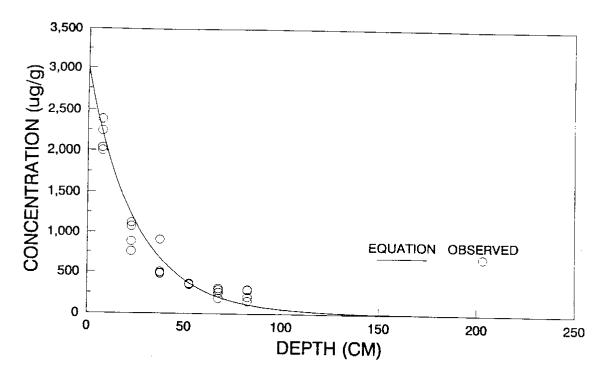


FIG. 5 Total elemental nitrogen with depth at Plymouth site.

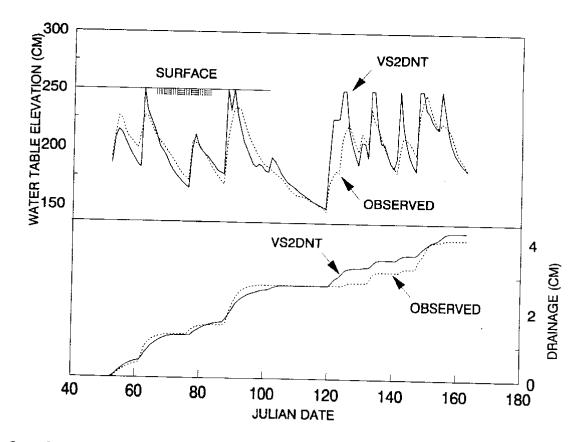


FIG. 6 Observed and calculated (VS2DNT) mid-point water table elevation and drainage volume.

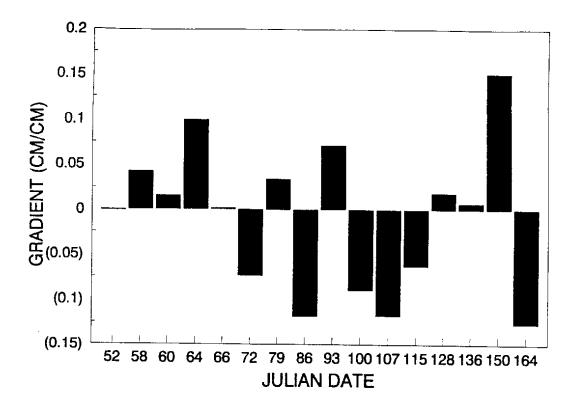


FIG. 7 Vertical hydraulic gradient at restrictive layer.

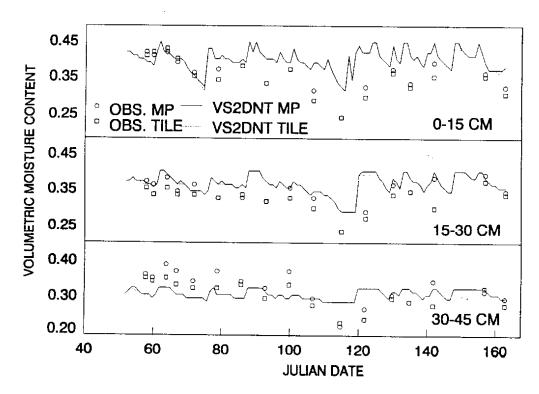


Fig. 8 Observed and calculated (VS2DNT) volumetric moisture content with time for three upper depths.

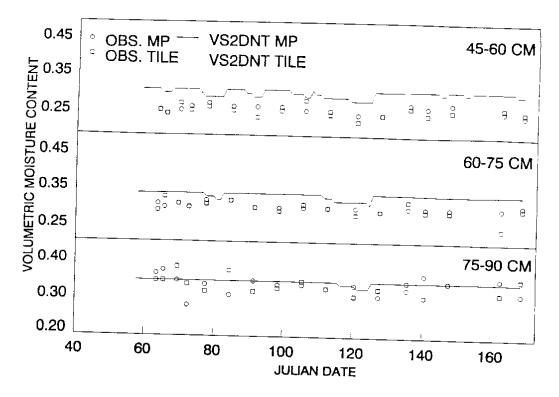


Fig. 9 Observed and calculated (VS2DNT) volumetric moisture content with time for lower upper depths.

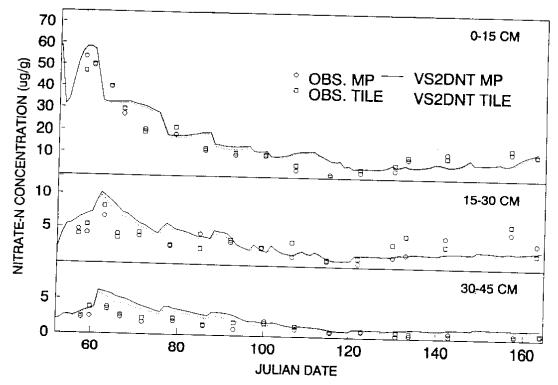


Fig. 10 Observed and calculated (VS2DNT) nitrate-N concentration with time for three upper depths.

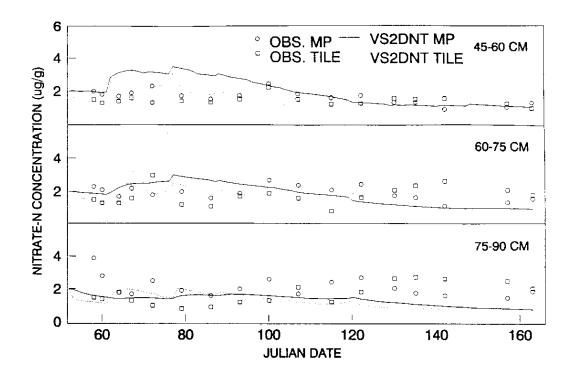


Fig. 11 Observed and calculated (VS2DNT) nitrate-N concentration with time for lower three depths.

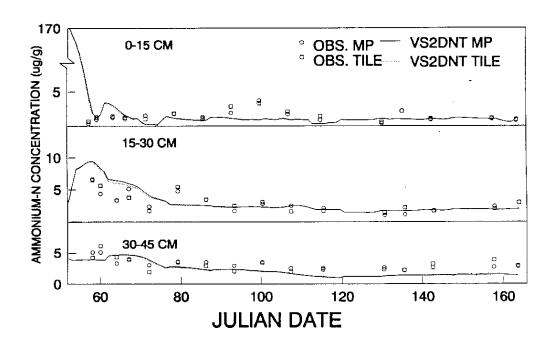


Fig. 12 Observed and calculated (VS2DNT) ammonium-N concentration with time for three upper depths.

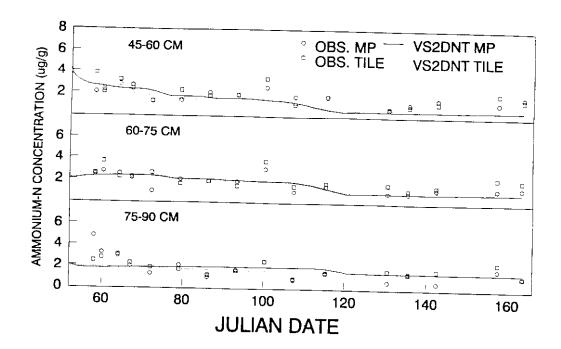


Fig. 13 Observed and calculated (VS2DNT) ammonium-N concentration with time for lower three depths.

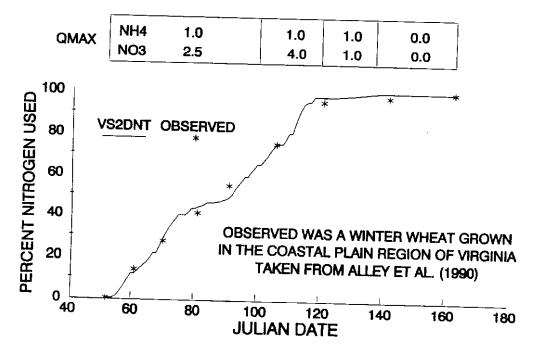


Fig. 14 Observed vs. calculated (VS2DNT) normalized nitrogen use by wheat crop with time. Observed was a winter wheat grown in the coastal plain region of Virginia taken from Alley et al. (1990). Figure also shows  $q_{\text{max}}$  values with time.

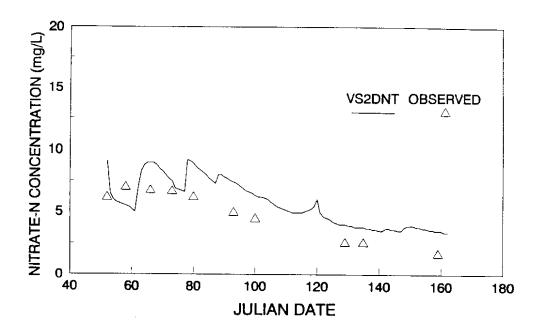


Fig. 15 Observed and calculated (VS2DNT) Drainage water nitrate-N concentration with time.

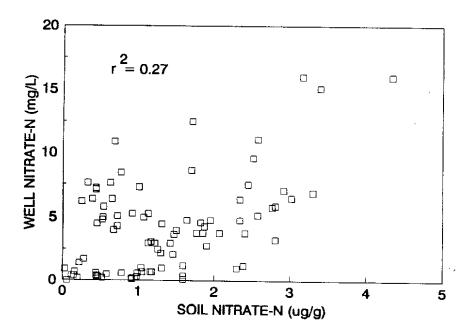


Fig. 16 Soil vs. well nitrate-N concentration.

Crop: corn, planted Apr. 15

Location: Aurora, NC

Simulation time: March 1 - Sept. 1 (190 days)

Rainfall, PET and root growth: from 1975 season

Drain spacing: 7.5 m

Water management treatments:

Free Drainage

**Controlled Drainage** 

**Fertility Treatments:** 

SINGLE - 150 kg/ha Apr. 15

SPLIT - 50 kg/ha Apr. 15, 100 kg/ha May, 22

Fig. 17 Simulated conditions used for the example problem.

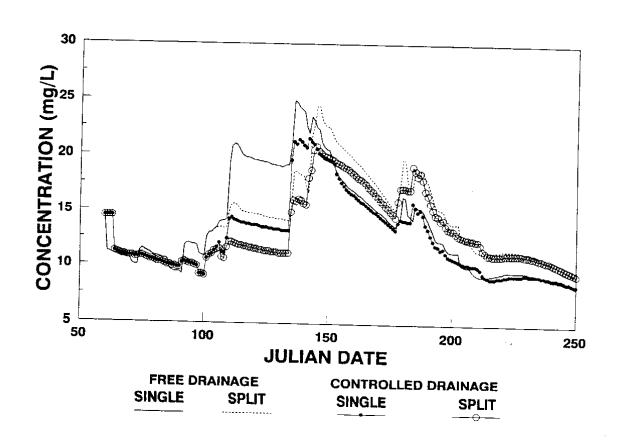


Fig. 18 Drainage water nitrate-N concentrations with time for the treatments.