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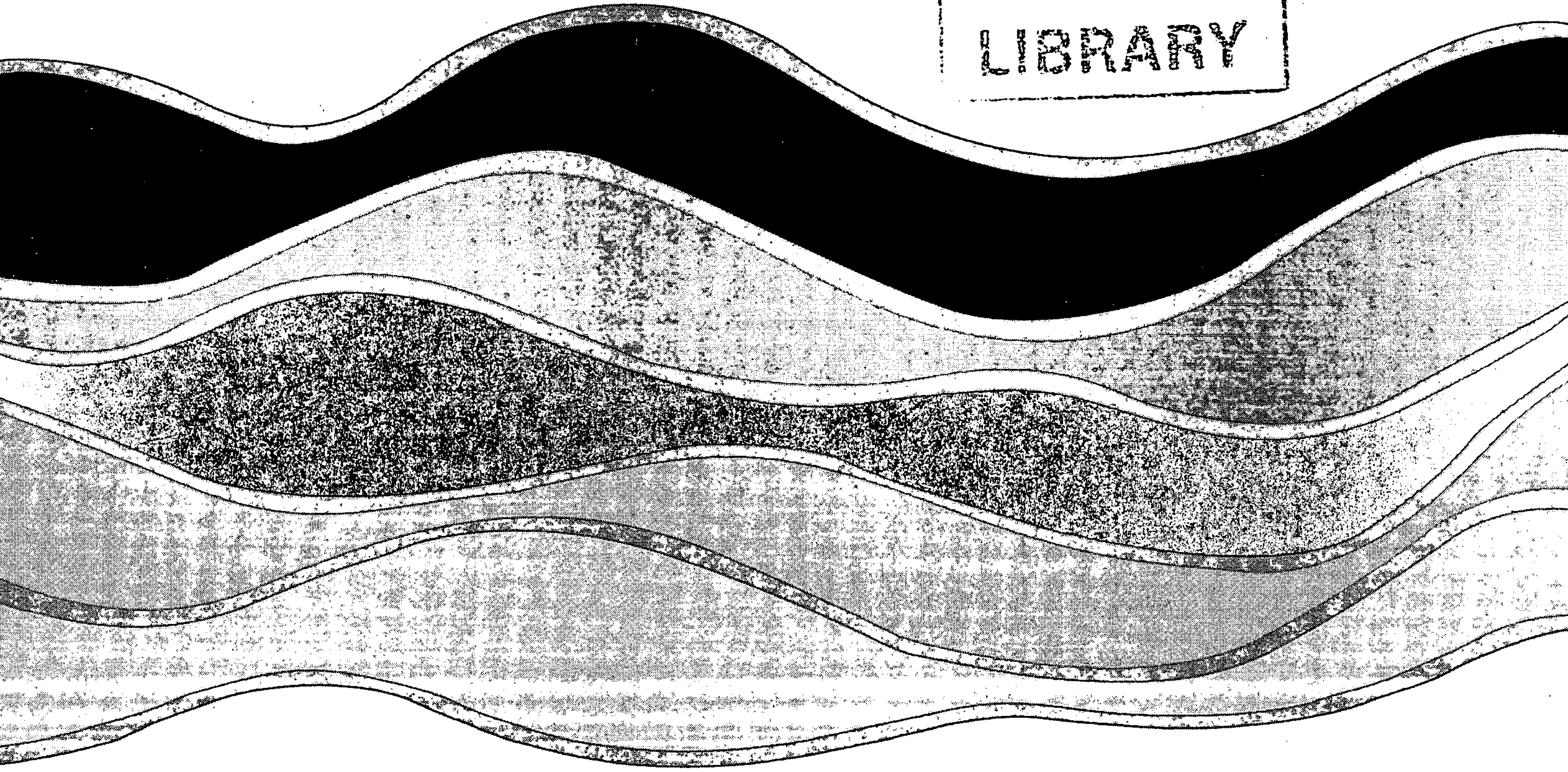

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MANAGEMENT PERSPECTIVE

The Root Zone Water Quality Model (RZWQM) developed by the U.S. Agriculture Research Service was evaluated for subsurface drain volumes and nitrate concentrations in the drain flow in an experimental plot under free drainage management. The results of the evaluation demonstrated that RZWQM can simulate physical and chemical processes in the root zone of crops. The results of the evaluation of the model are reported here. The biological component of the model was not evaluated at this time.

SOMMAIRE A L'INTENTION DE LA DIRECTION

Le modèle de qualité de l'eau de la rhizosphère (Root Zone Water Quality Model ou RZWQM) du Service de recherche agricole des États-Unis a été appliqué à l'évaluation du volume d'eau et de la concentration du nitrate dans des drains souterrains à écoulement libre situés dans une parcelle expérimentale. Les chercheurs parviennent à la conclusion que le modèle peut simuler les processus physiques et chimiques qui ont leur siège dans la rhizosphère de sols cultivés. Cet article présente les résultats de l'évaluation du modèle. La composante biologique n'a pas fait l'objet d'une évaluation.

ABSTRACT

Evaluation of the subsurface drain volumes and the nitrate concentrations in the drained water, in a field plot, was conducted by using the Root Zone Water Quality Model (RZWQM), version 3.5. A Parameter Estimator (PEST) model was used to calibrate the subsurface tile drain flow parameters and the nitrate parameters of the RZWQM, using data measured in a field plot under free drainage management.

The discrepancy between the simulated average tile drain flow (0.0274 cm/day or 6.03 m^3/day) and the measured drain flow (0.0190 cm/day or 4.2 m^3/day) was about 31%. The discrepancy between the simulated average nitrate concentration (15.5 mg/L) and the average measured nitrate concentration (12.9 mg/L) was about 16.8%. Both the simulated average tile drain flow and the simulated average nitrate concentrations were higher than the measured values. However, the reported discrepancies are within acceptable ranges of accuracy.

RÉSUMÉ

Les auteurs ont évalué l'écoulement d'eau et la concentration de nitrate dans l'eau, dans des drains souterrains situés dans une parcelle expérimentale, au moyen de la version 3.5 du modèle RZWQM (Root Zone Water Quality Model). Ils ont utilisé un modèle d'estimation des paramètres (PEST) pour étalonner le RZWQM au regard des paramètres relatifs à l'écoulement et au nitrate; ils ont utilisé, pour cela, des données prélevées sur une parcelle en régime d'écoulement libre

L'écart entre l'écoulement moyen simulé (0,0274 cm/jour ou 6,03 m^3/jour) et celui qui a été mesuré (0,0190 cm/jour ou 4,2 m^3/jour) est d'environ 31 %. L'écart entre la concentration moyenne simulée du nitrate (15,5 mg/L) et la concentration mesurée (12,9 mg/L) est d'environ 16,8 %. Les résultats simulés du volume et de la concentration sont tous deux supérieurs aux valeurs mesurées. Cependant, les écarts se situent à l'intérieur des valeurs acceptables.

INTRODUCTION

Models are useful tools for studying complex natural phenomena. To advance the management of agricultural impacts on the environment and to achieve sustainable agriculture, there is a need for a model that can simulate the physical, chemical, and biological processes in the root zone. Such a model has to be sensitive to the effects of management practices. The Root Zone Water Quality Model (RZWQM) was developed by the U.S. Agricultural Research Service to meet such needs.

Reliable modelling results depend on the model structure, assumptions and the accuracy of model parameter estimations. Most importantly, models require to be calibrated against a set of standardized data or actual measured data before they can be used for simulation and testing of management practices.

Before starting the calibration process the user should identify which parameters need to be calibrated. The process of determining which model parameters cause the greatest changes in the model's output is termed sensitivity testing of the model. This testing is an important step in determining the most sensitive parameters that play important roles in the calibration processes.

The objective of this study is to evaluate the applicability of the RZWQM to a field plot under free drainage management. The calibrated RZWQM will be used for our subsequent study on field plots under controlled drainage management.

The Study Area

The study area designated as Shanahan farm is located in the Township of Maidstone, County of Essex, Province of Ontario. The site consisted of two plots (Figure 1). The first plot has a free drainage setup and the second plot has a controlled drainage setup. The area of the free drainage plot is 2.2 ha and the controlled drainage plot has an area of 2.4 ha. This study focused on the free drainage plot.

The RZWQM requires certain physiographic input data. The data describe the study site where the simulation will take place. These data are the field site elevation above the mean sea level, and the topographic slope of the field. The elevation of the free drainage plot is 182 m above the mean sea level. The geographical location of the field measured clockwise from true north is 0.698 radians. Its latitude is 0.737 radians and its slope in radians is 0.0798.

The RZWQM requires that the field is divided into a number of soil horizons also called layers. The field plot used for this study was divided into two horizons. The first horizon extended 30 cm from the surface. The second horizon extended from 30 cm to 150 cm from the surface. However, the availability of field data for the soil horizon was only from the surface to 60 cm depth. No measurement was conducted for soil horizons between 60 and 150 cm. Consequently, data from the 30-60 cm horizon were assumed to be representative for the layer of 30 -150 cm.

The tile drains layout with a free drainage setup is shown in plot 2 of Figure 1. The instrumentation on the free drainage plot has been reported elsewhere (Tan et al., 1996). Plot 2 is drained by five tile drains having an average diameter of 102 mm, at an average depth of 76 cm and their average spacing is 10 m. The plot was planted with soybean in 1995.

The soil classification in the study area is Brookston Clay. Table 1 shows some of the major soil properties for the study area.

Table 1: Selected soil properties for the free drainage plot

Horizon (No.)	Depth (cm)	Bulk density (g/cm^3)	Particle density (g/cm^3)	Porosity (m^3/m^3)	Particle size distribution [%] sand	silt	clay
1	0 - 30	1.38	2.59	0.46718	22.7	22.5	54.8
2	30 - 150	1.38	2.66	0.48120	20.1	15.5	64.4

Methods and procedures

The Root Zone Water Quality Model

The Root Zone Water Quality Model (RZWQM) version 3.5 was developed by USDA-ARS (1992; 1996). RZWQM consists of three independent programs: (1) the numerical grid generator, (2) the simulation program, and (3) the output report generator.

The RZWQM was developed to simulate the physical, chemical and biological processes at the root zones. Major processes of the RZWQM included movement of water, nutrient and water uptake by plants, pesticide degradation and transformation above and within the soil root zone, and the plant growth. The primary use of the model is to study the effect of various farming practices on both surface and subsurface water quantity and quality.

The RZWQM requires a large amount of input data which include the soil physical characteristics, soil chemistry, hydraulic properties, precipitation data, evapotranspiration rates, wind speed, relative humidity, minimum and maximum daily temperatures and solar radiation, plant species, plant grow index, types of fertilizers and pesticides, types of application, and biomass.

The daily tile flow data in Julian days, from 128 to 365, at the study site for 1995, were used.

Most of the climatic data can be calculated by the model if it is not measured except for the minimum and maximum daily temperature. In this study the climatic data were measured and available for the calibration of the model. All the climatic data were daily values except precipitation data used in this study, which were hourly values. The precipitation data were converted to a breakpoint data format for each storm. The breakpoint data format is the cumulative precipitation values which are plotted against the time duration of the storm. An example of the breakpoint plot of precipitation is presented in Figure 2. Note that, due to the model's setup, the input of precipitation data has to be in imperial unit. The breakpoint is chosen at an abrupt change in slope, i.e., the rate of change in storm intensity. It should also be noted that the input time steps of precipitation data have to be in hourly time steps. It is preferable that the time steps be in minutes. The meteorological data were recorded at the Agricultural Experimental Station, Agriculture and Agri-Food Canada, located in Woodslee. The station is located about 2 km from the study site. The climatic data are assumed to be representative of the study site.

Model Independent Parameter Estimation (PEST)

This section discusses the Independent Parameter Estimation Model (PEST), which is a non-linear parameter estimation model that allows the user to undertake parameter estimation and/or interpretation using a particular model, without the necessity of having any changes to the parent model structure (Doherty, 1994).

PEST will adjust model parameters until the fit between model outputs and laboratory or field observation is optimized in the weighted-least-squares sense. PEST can perform this task for any model that can read its input data file from an ASCII text file and writes the output of its calculations to an ASCII output file.

In order to have PEST optimize the parameters, the parameters first need to be identified. This was done for RZWQM by building a template file showing which parameters are free for adjustment. After building the template file, two utility programs (PESTCHEK and TEMPCHEK) are used to check the syntactic correctness and consistency of the template. Each parameter is identified by a unique name up to four characters long and can be referenced to one or more times in the template file. Any parameter can be fixed during the optimization process.

Upper and lower bounds for the adjusted parameters are required. This instructs PEST about the range of allowable values that a parameter can reach.

Instructions are provided to PEST in order to track the required RZWQM output file. For each model output file PEST requires an instruction file detailing how it can find the observations in the output file. The instruction file can be checked for syntactic correctness and consistency using the utility programs of PESTCHEK and INSCHEK.

Once interfaced with the model, PEST's role is to minimize the weighted sum of squared differences between the model-generated values and the field measured values. This is referred to as the "objective function".

The three files required for PEST are given below.

1. Template files, one for each model input file that the PEST must write prior to a model run.
2. Instruction files, one for each model output file that the PEST must read after a model run.
3. PEST control file that supplies PEST with the names of all template and instruction files together with the model input/output files to which they pertain. It is also required to provide the PEST with the model name, initial parameter estimates, and data records, to match the model output. PEST uses a non-linear estimation technique known as the "Gauss-Marquardt-Levenberg parameter", named after Marquardt (1963). This is a parameter estimation method. This process requires that an initial set of values of parameters be supplied to start off the optimization process. The optimization is an iterative convergence towards the interactive improvement of initial parameter values or the objective function minimum. The algorithms of this process are not repeated here because the equations are lengthy to list. This method is able to estimate parameter values using fewer iterative runs than any other parameter estimation method (Doherty, 1994). The numbers of PEST variables that control the implementation of the Gauss-Marquardt-Levenberg method (Doherty, 1994) of optimization need to be given. Further details related to the PEST algorithms can be found in the PEST manual (Doherty, 1994).

Results and Discussion

The literature survey showed that parameters such as vertical and lateral saturated hydraulics properties are most sensitive to the drain flow. Walker (1994, 1996) and Singh et al., (1996) conducted a sensitivity analysis for the earlier version of RZWQM, the version 2.5. They found that the most sensitive parameters were both the lateral and vertical saturated hydraulic conductivities. The automatic calibration was carried out to determine the optimum value for the saturated hydraulic conductivity. The lateral and vertical hydraulic conductivities were assumed to be equal in this study. Other sensitive parameters considered in this study were the infiltration and leakage rates.

The discrepancy between the average measured drain flow (0.019 cm/day) and the simulated average drain flow (0.0274 cm/day) was about 30%. Figure 3 shows a plot of the simulated and the measured daily tile flow for 1995. The reasons for such a discrepancy may be the time step of precipitation input data, the length of data record used in the calibration process, and the fact that some of the required parameters were assumed to be equal to the default values provided with the model. For example, some of the modified Brooks-Corey (1964) parameters were assumed. The Brooks-Corey parameters are the soil physical and hydraulic properties showing the soil water-content-matric suction relationship and the unsaturated hydraulic conductivity-matric suction relationship. The soil water-content-matric suction relationship and the unsaturated hydraulic-conductivity-matric suction relationship are repeated here for convenience.

(a) The soil water content vs. the matric suction relationship is represented by:

$$\theta(\tau) = \theta_s - A_1\tau \quad ; \quad \tau \le \tau_b$$
$$\theta(\tau) = \theta_r - B\tau^{-\lambda} \quad ; \quad \tau \ge \tau_b \tag{1}$$

where θ = volumetric soil water contents (cm^3/cm^3),

τ = matric suction (cm, $\tau = |h|$, where h is the capillary presure head),

θ_s = saturated soil water content (cm^3/cm^3),

θ_r = residual water content (cm^3/cm^3), and

τ_b = air-entry (drying of soil) or bubbling suction (cm).

A_1, B, and λ are constants. The constant B is not an independent parameter. It is determined from other parameters by the condition of continuity at $\tau = \tau_b$. When A_1 is set equal to zero, Equation (1) is reduced to the Brooks-Corey model.

(b) The hydraulic conductivity vs. matric suction relationship is expressed as:

$$K(\tau) = K_s \tau^{-N_1} \quad ; \quad \tau \leq \tau_{bK}$$

$$K(\tau) = C_2 \tau^{-N_2} \quad ; \quad \tau > \tau_{bK} \qquad (2)$$

where K = hydraulic conductivity (cm /hr),

K_s = field-saturated hydraulic conductivity (cm /hr), and

τ_{bK} = air-entry (soil drying) or bubbling suction for this function (cm), which may equal τ_b introduced above.

N_1, N_2, and C_2 are constants. Again, C_2 can be computed from other constants at τ_{bK}. The technique of estimation of the soil hydraulic properties can be found in the Technical Documentation of RZWQM (USDA-ARS, 1992; 1996).

The hourly precipitation time step was used in this study and might have affected the calibration process. Shorter time steps (preferably in minutes) of precipitation were recommended (Walker, 1997). This is particularly sensitive for the study of a small land area (2.2 ha) like Shanahan farm. The length of climatic data record could be another factor that contributed to the discrepancy. Three years of climatic data is a recommended minimum for calibration of an environmental model (Donigian, et al., 1991). In our study, only one year of climatic data was available.

Nitrate concentrations in the tile drain, measured on four different dates were used for the calibration of the RZWQM (Figure 4). The period covered spanned from the early spring to mid fall. These periods corresponded to the active periods of crop growth on the farm. The average measured nitrate concentration in the drain flow was 12.9 mg/L, and the simulated average nitrate concentration in the drain flow was 15.5 mg/L. The discrepancy between the of simulated average nitrate concentration and the average measured nitrate concentration was about 17 %. As shown in Figure 4, the simulated value of June 29, 1995 was 35% larger than the measured value. Perhaps this was due to the presence of rainfall on June 28 and 29 coupled with fertilizer residues. The amount of rainfall during this period was 6.9 mm. The fertilizer application date was on May 31, 1995. Since soybean fixed nitrogen during this growing period, there was more nitrate in the soil profile available for leaching.

Summary and Conclusions

Our results showed that the RZWQM has the capability to predict the drain flow with a reasonable accuracy. The model requires large amounts of input data in order to achieve good results. In our study, some of the data were not readily available. Thus, the default values provided by the model had to be used. The model can address many existing field conditions under free drainage. The current version of the RZWQM can not deal with the field conditions under controlled drainage. Testing of the RZWQM for field conditions under controlled drainage (Plot 1, Figure 2) was not evaluated at this time.

ACKNOWLEDGMENTS

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Figure 1. Study Area

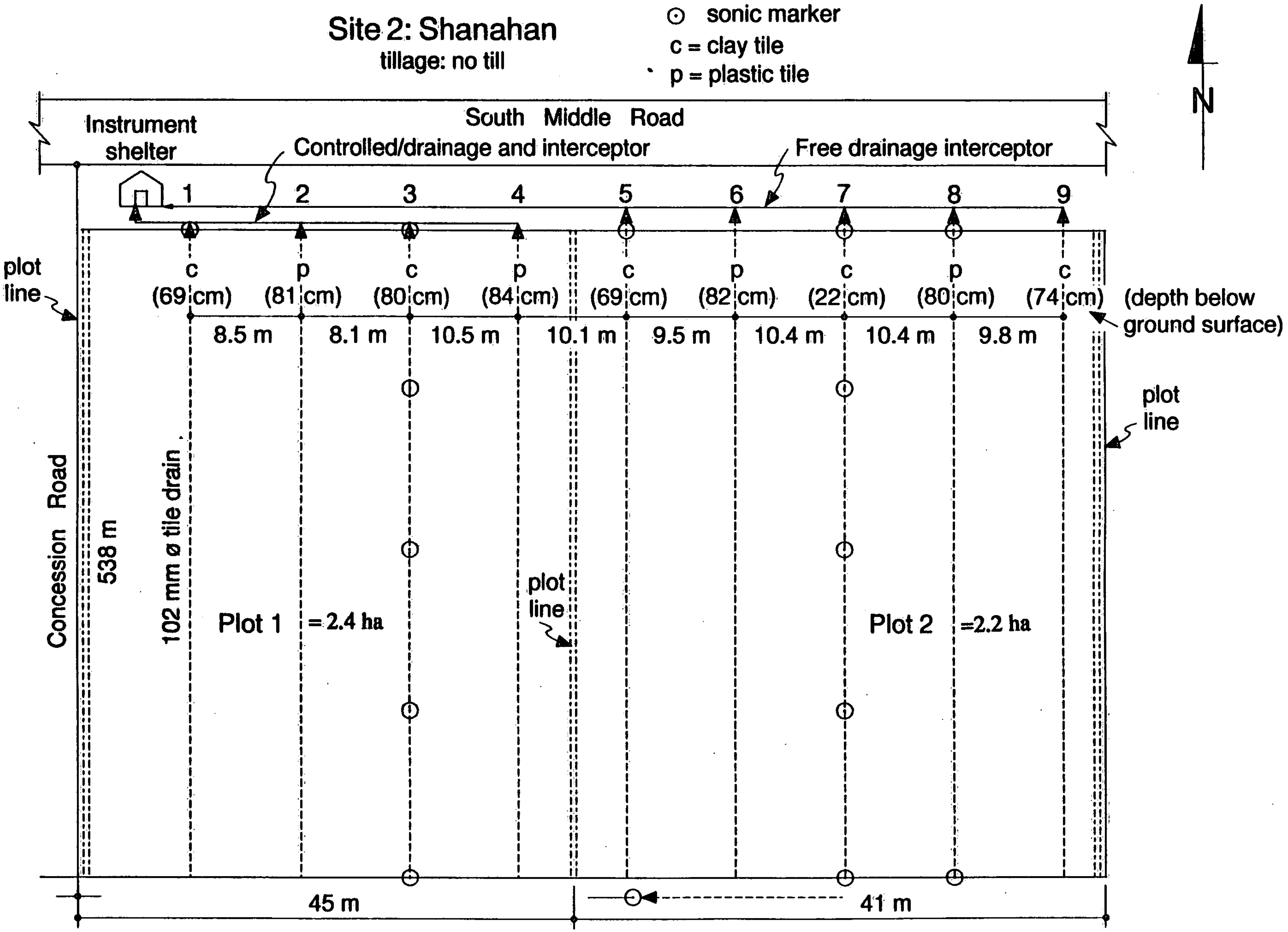


Figure 2. Precipitation breakpoint determination, julian day 14-15, 1995

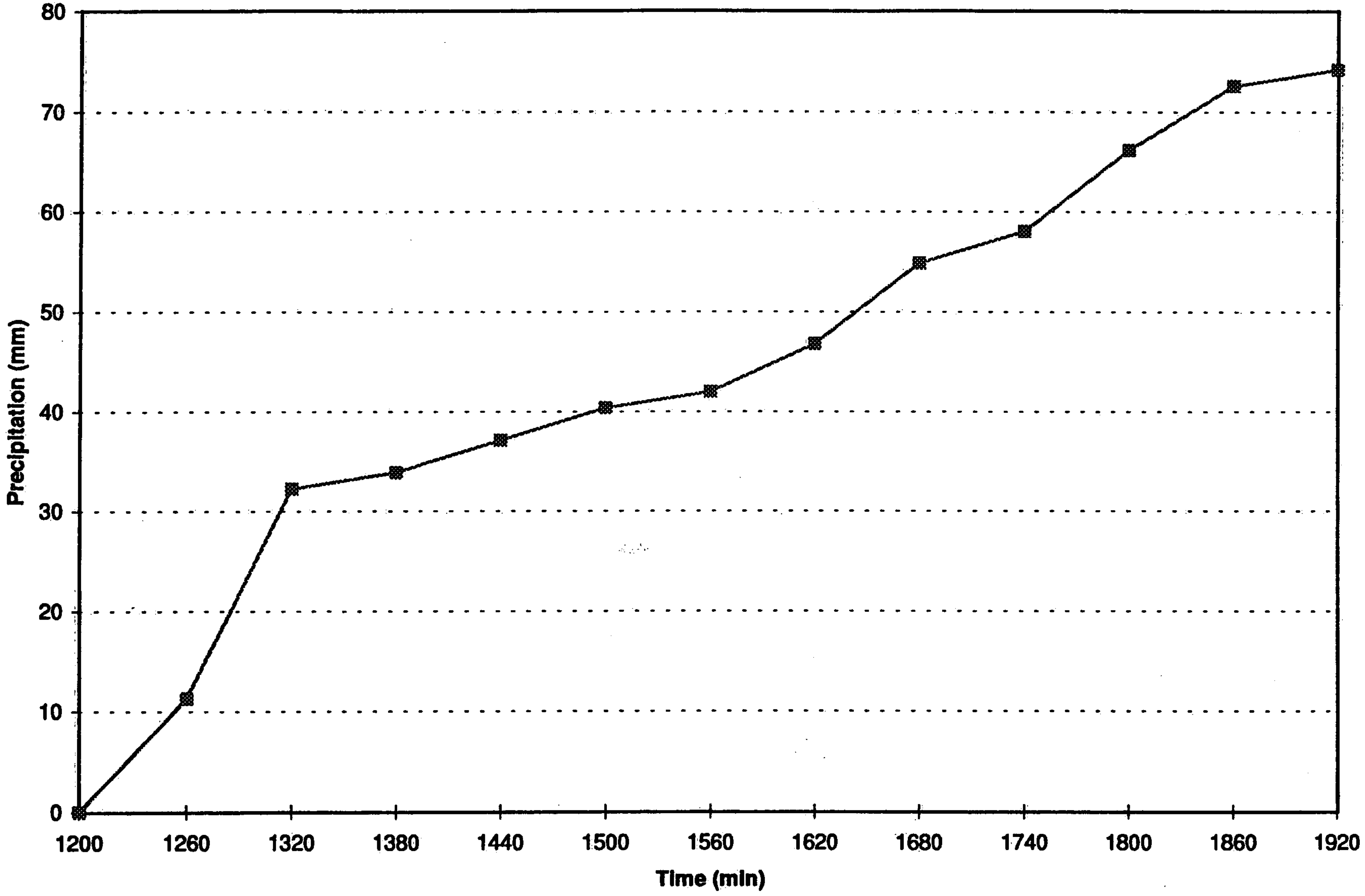


Figure 3. Relationships between the measured and simulated tile flow, 1995 (Shanahan Field Plot)

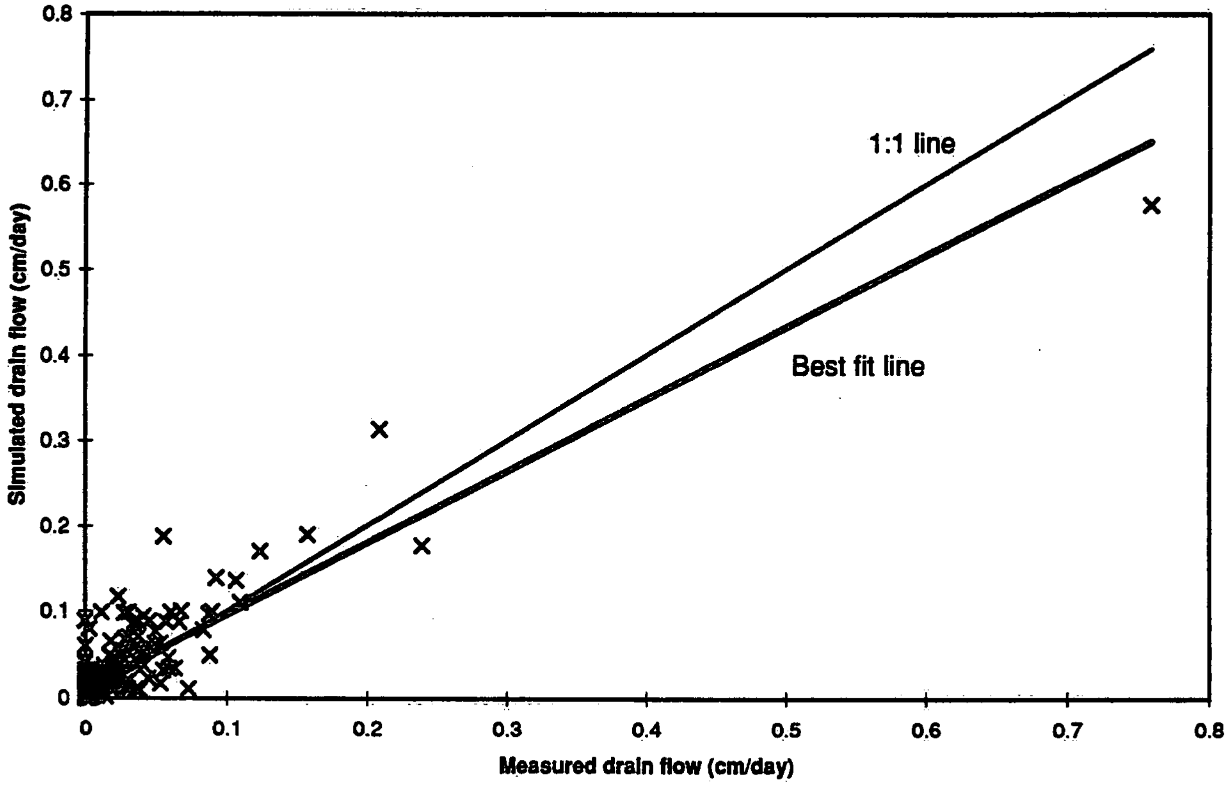
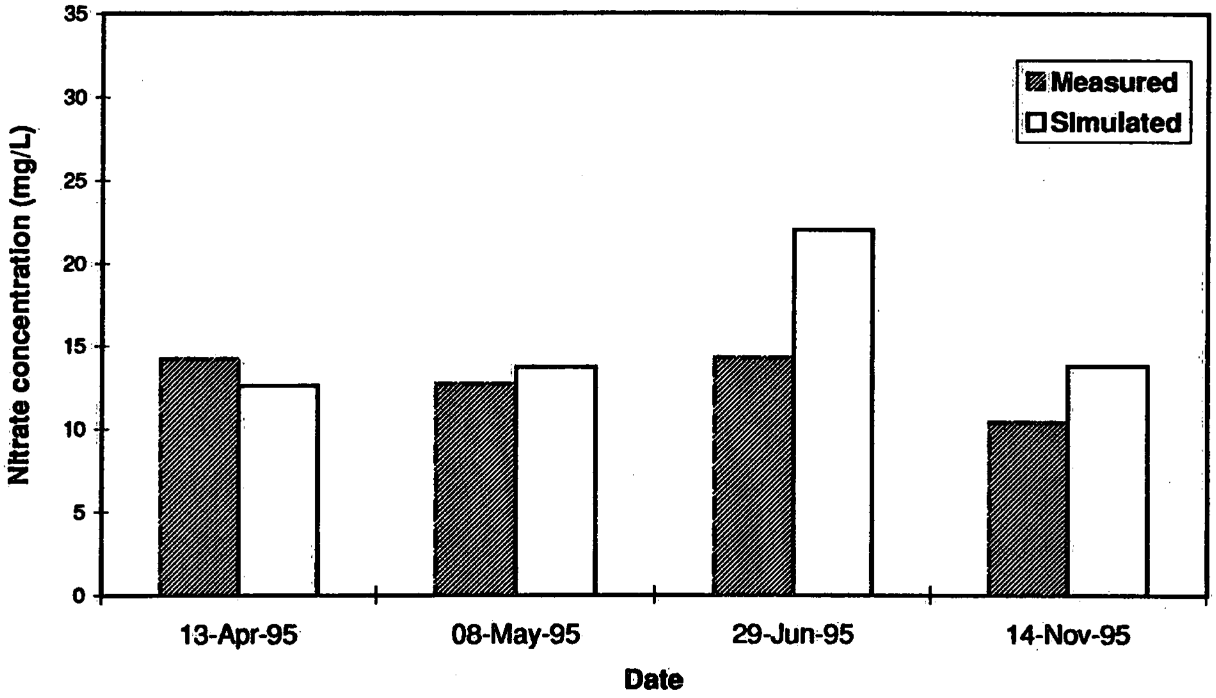
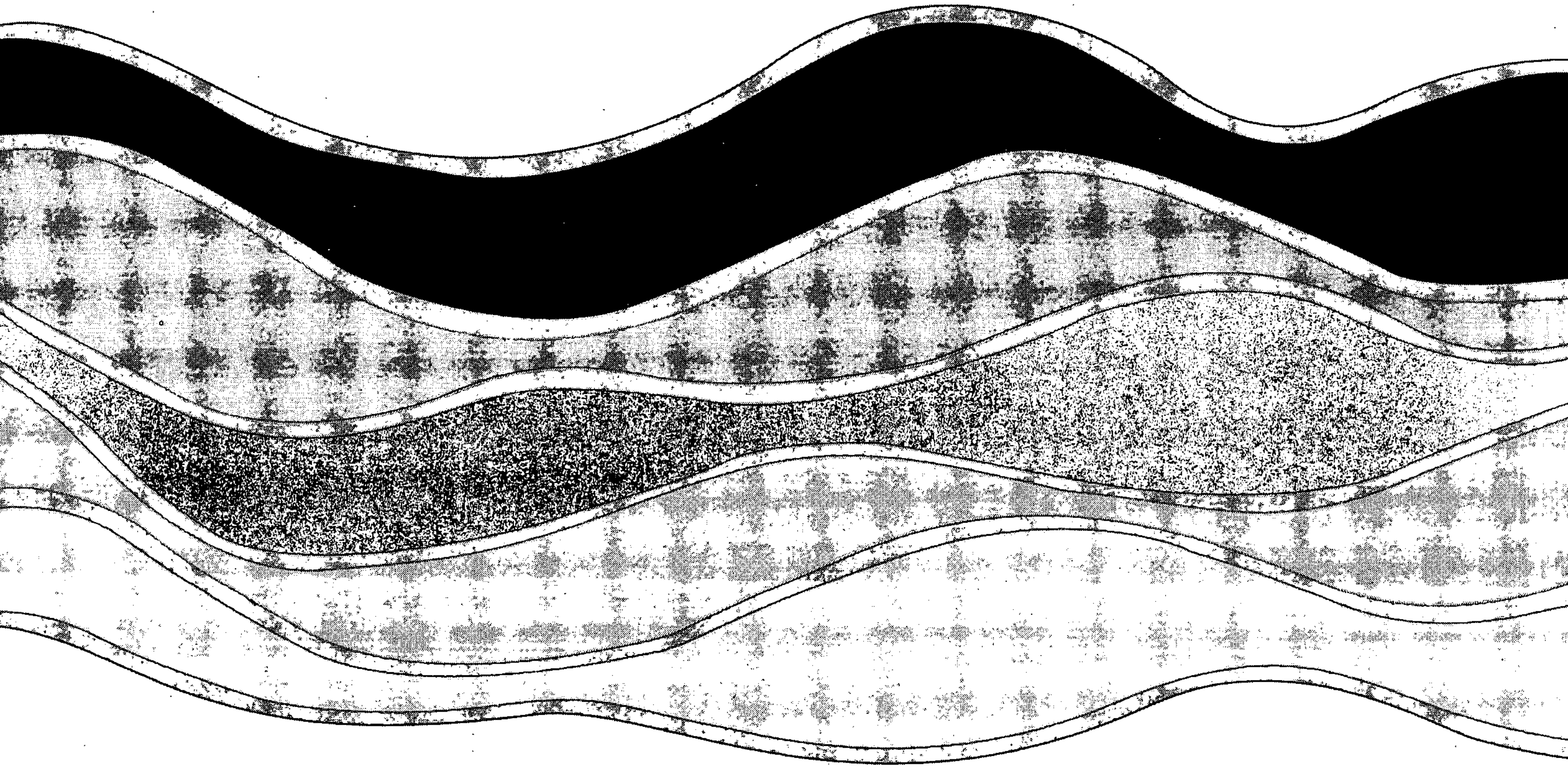


Figure 4. Measured and simulated nitrate concentration, 1995





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