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Modeling of the Fate and Agrochemical Movement Under Controlled Water Table Environment

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ABSTRAK

Kajian telah dijalankan untuk mengenal pasti keberkesanan amalan pengurusan paras air terhadap angkutan persekitaran dan kesan agrokimia. Satu kajian makmal dijalankan menggunakan tanah pasir berkolum yang terganggu bagi mengenal pasti angkutan dan kesan nitrat (NO_3), sejenis bahan kimia pertanian yang biasa diguna terhadap persekitaran bawah tanah yang dipengaruhi oleh kedalaman paras air terkawal. Tiga sampel kedalaman paras air terkawal yang digunakan ditetapkan, pada paras 0.25 m, 0.50 m dan 0.75 m dari permukaan dan rawatan penyaliran bebas (tiada kedalaman aras air terkawal). Satu model statistik mudah berasaskan analisis kepelbagaian regresi linear dibina menggunakan data eksperimen bagi menyerupai penurunan dan angkutan nitrat dalam tanah berkolum di bawah paras air yang berbeza. Model regresi dibina daripada pemboleh ubah yang terpilih termasuk kedalaman paras air dari permukaan, masa dan kedalaman tepu. Satu persamaan yang luas didapati daripada data eksperimen bersama dengan koefisien korelasi R^2=0.83. Prestasi persamaan ini diuji dengan menggunakan data eksperimen dan didapati keputusan daripada ujian tersebut memuaskan dan boleh diterima. Berdasarkan kepada keputusan tersebut, jelas ia menunjukkan paras air mempengaruhi perlakuan angkutan nitrat. Sebagai tambahan, penurunan paras kelikatan nitrat diperoleh daripada rawatan paras air. Keputusan ini mengesyorkan bahawa tidak mustahil melakukan degradasi pada bahan kimia dan biologi bagi menurunkan angkutan nitrat dengan mengawal kedalaman paras air.

ABSTRACT

The study was undertaken to investigate the effect of water table management practices on the environmental transport and fate of agrochemicals. A laboratory based study using disturbed sand soil columns was conducted to investigate the transport and fate of nitrate (NO_3), a commonly used agricultural chemical, to the underground environment as effected by controlled water table depths. Three controlled water table depths set as 0.25m, 0.50m, and 0.75m from the surface and free drainage treatment (no controlled water table depth) were used. A simple statistical model based on multiple linear regression analysis was developed using experimental data to simulate reduction and transport of nitrate in soil columns under different water table depths. The regression model was developed from selected physical variables including water table depth from the surface, time, and saturated depth. An imperial equation was obtained from the experimental data with a correlation coefficient of R^2 = 0.83. The performance of this equation was tested using experimental data and it was found that the output from this equation is acceptable and satisfactory.

According to the simulated and observed results, it was clearly shown that the water table depth affects the characteristics of transport nitrate. In addition significant reduction in nitrate concentration was achieved through different water table treatments. The results suggest it is possible to promote biological and chemical degradation to reduce nitrate transport by controlling water table depths.

Keywords: Water table depths, statistical model, nitrate concentration

INTRODUCTION

Ground water quality degradation in rural areas is frequently attributed to agricultural production practices involving the use of fertilizers and pesticides for sustaining productivity. A fraction of farm chemicals moves to surface and ground water reservoirs by mass flow and diffusion processes .The accrual of soluble agricultural chemicals, particularly nitrate NO_3 to ground water is a natural process and source of potential degradation of ground water (Prunty and Montgomery 1991). At present, ground water contamination from agricultural non-point sources has become a major environmental concern and awareness, which is needed to protect ground water quality. A variety of interacting physical, chemical, and biological processes determined how far agrochemicals will move in the soil, how long it will persist in the environment, and at what concentration it will appear in water resources system. Recently researchers have been investigating the possibility of developing best management practices to protect water resources from agrochemical pollution. A few studies have been reported in evaluating the ability of water table management practices to reduce negative impact on water quality (Evans *et al.* 1989; Belcher 1989). Because of high costs and heterogeneities in soil properties caused by spatial and temporal variations in field experiments, most research has been performed in laboratories, usually in repacked soil columns or large field lysimeters.

To assess the impact of agrochemicals on water quality, predicting the transport and the fate of agricultural chemicals released into the environment it is necessary to minimize adverse impacts and optimize positive impacts. The complexity of agricultural chemical transport and the fate processes encourage the development and use of computer and statistical models for assessing the movement of chemicals in different pathways and under different climatological, geological, and management scenarios. Due to the complexity and costs of field experimental procedures, the use of statistical and computer modeling as an alternative is essential in conducting research in this area. In recent years, substantial progress has been made in the use of modeling as a tool to integrate processes for predicting agricultural chemical behavior in the environment.

Various contaminate transport models have been developed under different management practices for monitoring agrochemical behavior in an environmental system (Wagenet 1990). Regression models are examples of empirical models used as a tool for predicting the concentration of agrochemicals in water system (Druliner *et al.* 1996) . Based on laboratory experiment studies, the specific objectives of this study was to investigate the effect of various water table depths on the transport and fate of nitrate to subsurface environment and to create a statistical model to simulate the nitrate reduction under these conditions. Also the model validation was done by comparing the predicted outputs from the model with the observed data to study the effect of water table depths on the predicted outputs.

MATERIALS AND METHODS

Soil Preparation

This research was undertaken to investigate the effect of water table levels on agricultural chemical transport to underground environment, specifically nitrate transport and transformation, and to identify water table management strategies that can help to reduce the potential of agricultural chemical (nitrate) pollution to both surface and ground water. The main factor considered in this research is the effect of water table levels on nitrate movement. To achieve the overall objectives, this study consists primarily of laboratory work and then a statistical model to simulate the studied problem. The laboratory experiments were conducted on a column system. The columns were constructed from PVC pipes with a 30 cm diameter and 1-meter high welded with thin iron sheet at one end. The columns were equipped by two holes at the bottom of each column for collecting water samples and to maintain water table levels at the desired depths in each column. A water supply system was attached to the side of columns to monitor water table depth (*Fig. 1*). The soil used in the column experiments

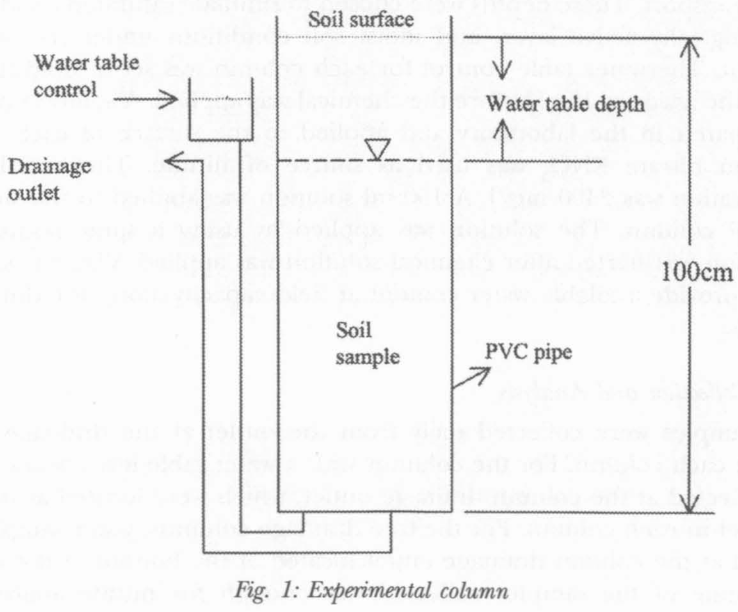

Fig. 1: Experimental column

was disturbed sandy soil collected from the field. The soil samples were air-dried and sieved through 2 mm sieves before being placed in the columns. Selected physical properties of the soil used in this study are listed in Table 1. A total of four columns were used in this study. To approximate the bulk density of the original soil 1.35 g/cm^3, an equivalent weight of soil was used to make the soil volume to each column.

TABLE 1
Summary of soil physical properties used in the study

Soil property	Measured values
Silt (%)	3.98 %
Clay (%)	1.02 %
Sand (%)	95 %
Coarse sand (%)	30.70 %
Medium sand (%)	27.73 %
Fine sand (%)	25.20 %
Very fine sand (%)	11.8 %
Bulk density (g/cm3)	1.35 g/cm3
Hydr. Conduct (cm/sec)	0.0855 cm/sec

Water Table Experiment

Three control water table depths set as 0.25m, 0.50m, 0.75m from the surface and free drainage treatment (no control water table) were conducted in the column experiments to evaluate the effect of different water table depths on nitrate transport. These depths were chosen to simulate saturated conditions in the biologically active layer, and moist soil conditions under free drainage treatment. The water table control for each column was set to hold the water table at the assigned level before the chemical was applied. A solution of nitrate was prepared in the laboratory and applied to the surface of each column. Potassium nitrate KNO_3 was used as source of nitrate. The initial nitrate concentration was 2400 mg/l. A 150 ml solution was applied to the surface of each soil column. The solution was applied by using a spray bottle. Water application was started after chemical solution was applied. Water was applied daily to provide available water content at field capacity along the duration of the study.

Sample Collection and Analysis

Water samples were collected daily from the outlet at the drainage control point on each column. For the columns with a water table level, water samples were collected at the column drainage outlet, which were located at the water table level in each column. For the free drainage columns, water samples were collected at the column drainage outlet located at the bottom of the column. The volume of the samples collected was enough for nitrate analysis. The collected water samples from each column drainage outlet were analyzed to develop nitrate concentration curves for each water table depth. All water samples were analyzed immediately for nitrate concentration using a distillation method.

Statistical Evaluation Methods

In this study a simple statistical model based on multiple linear regression analysis as described by SPSS statistical package Version 10.0.5 and data collected from the experiments were used to evaluate reduction and transport of nitrate in soil columns with different water table depths. An empirical regression model was developed from selected variables including the depth of water table from the surface, time, and saturated depth (range of saturated conditions). In developing the regression model, the interactions between the variables were considered. Several statistical evaluation procedures were used to test the performance of the model (Addiscott and Whitmore 1987). These methods included mean error ME, root mean square error RMSE, correlation coefficient r, Thiel's coefficient U, and coefficient of determination R^2.

RESULTS AND DISCUSSION

Model Development

An imperial regression model was developed to simulate the reduction in nitrate concentration under different water table depths. The effective variables governing the studied phenomenon were considered in the model building. The model independent variables were selected based on the higher correlation coefficient with the dependent variable (r = 0.91). The general form of the regression model was expressed as:

$$\text{Log } y = -1.424 - 1.406\, T\, D\, D^2 - 1.469\, T\, S\, T^2 + 2.870\, S\, T^2 - 7.864\, D\, S\, S^2 - 9.503\, T^2 D^2 S^2 + 0.630\, D\, T^2 + 2.096\, D + 1.095\, T \quad (1)$$

where:

y = predict Nitrate concentration, (mg/l).
T = log time after application, (day)
D = water table depth from the surface, (meter)
S = saturated depth, (meter)

Equation (1) is the final form of the proposed model, which was obtained from the data of the experiment. The coefficient of determination (R^2) of the proposal model was significant and relatively high (R^2 =0.83) with standard error of 0.156. The coefficients of the regression model are given in Table 2. The results of t-test indicated the statistical significance of the independent variables on the dependent variable (t_{crit} =1.64 at 0.05level) as shown in Table 2.

TABLE 2
Parameter estimates for the final regression model

Predictor	Coefficient	Standard error	t-ratio	$t_{crit,0.95}$	R^2
Constant	-1.424	0.251	-5.67	1.64	0.83
TDD2	-1.406	0.273	-5.14		
TST2	-1.469	0.165	-8.90		
ST2	2.87	0.428	6.70		
DSS2	-7.864	2.118	-3.71		
T2D2S2	-9.503	0.923	-10.2		
DT2	0.630	0.091	6.89		
D	2.096	0.275	7.63		
T	1.095	0.222	4.93		

The high value of R^2 indicated that the regression model was appropriate to explain the relationship between these variables. The value of R^2 0.83 indicates that 83% of the variation in the dependent variable is explained by the regression variables in the model. This information is quite useful in assessing the overall accuracy of the model.

Model Verification

The verification process involves comparison between model predicted and observed data, preferably those not used in the model building process to achieve the best possible match of simulated outputs with observed data (Donigian 1983). For the proposed model, the verification process was conducted by comparing the regression model output with the data collected based on laboratory experiments. Comparison between simulated and measured results is shown graphically in *Fig. 2*. The results show satisfactory agreement between simulated and measured data. For the verification of this model, a best-fit regression model with $R^2 = 0.81$ was obtained for the relationship between simulated nitrate concentration and measured data. It is noticed that there is no significant difference in R^2 between the verification and the developed model. Careful visual observation of the best-fit line for the pooled data (*Fig. 2*) revealed that few points at the end of the best-fit line dominate the slope of the best-fit line. Otherwise, the best-fit line passing through rest of the data (excluding few points on the extreme left) provided a slope much closer to the 1:1 line (t-ratio = 0.46 compared to t-crit =1.67 at 0.05 significance level). The scatter of measured and simulated data on the developed model gives a good simulation to observed under study conditions. This statistically reasonable agreement between the measured and modeled results suggests that the model performed well.

Comparison with Experimental Results

The results of the experiments indicated that nitrate had different concentration curves depending upon the water table depths. Therefore the verification of

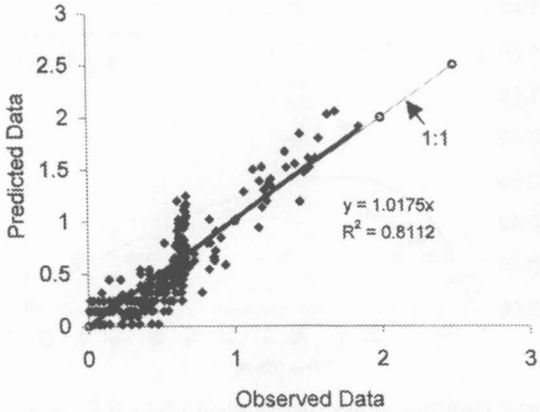

Fig. 2: Compassion between predicted and observed NO_3 concentration

the model was implemented upon all water table depths. A comparison of observed and model simulated nitrate concentration under 0.25 m, 0.50 m, 0.75 m and free drainage water table treatments are shown in *Figs. 3* to *6.* It is apparent from these figures that there is relatively good agreement between simulated and measured data. The nitrate concentration for 0.25 m, and 0.50 m, 0.75 m water table depths were lower compared to that under free drainage water table treatment. A similar trend was found in the simulated results from the model. These results suggest that more nitrates have been denitrified, especially in 0.25 m and 0.50 m water table depths. The saturated conditions in 0.25 m, and 0.50 m water table depths and anaerobic conditions, which are usually associated with high water content, may create the potential for more nitrate denitrification compared to the free drainage water table depth. In the column with free drainage water table depth, nitrate had to travel longer through the unsaturated zone where less denitrification would occur because of the lower degree of saturation. In the column with 0.75 m water table depth the saturated and anaerobic conditions may not have been sufficient to produce similar results for 0.25 m and 0.50 m water table depths. As a result, denitrification in the 0.75 m water table depth and free drainage columns would be lower compared to that in 0.25 m and 0.50 m water table columns. It appears that the different water table depths provide different degrees of saturation condition associated with different degree of anaerobic conditions, which is resulting in different degradation rates for nitrate. These observations agree with that reported by Jebelle and Prasher (1995) who found that shallow water tables would cause a faster degradation of nitrate. They assumed that the soil water content may affect soil chemical, physical and microbiological activity which would influence soil biodegradability. In addition, under saturated conditions, degradation capacity could be significantly increased. Several statistical parameters of the observed and simulated concentration curves were calculated. These statistical measures are used as indicators of the extent at which the

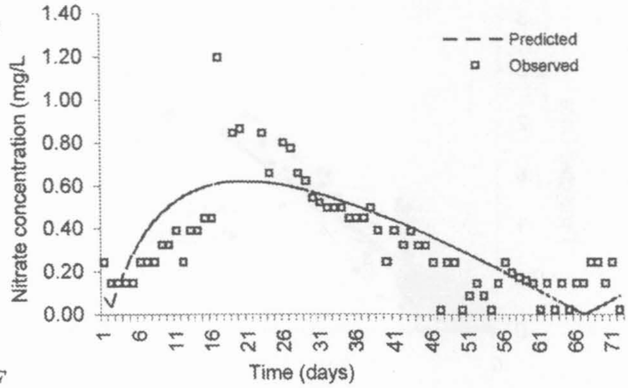

Fig. 3: Observed and predictive nitrate concentration under 0.25 m water table treatment

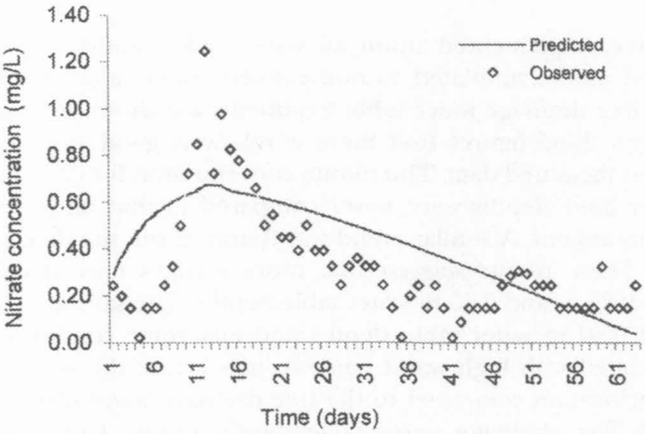

Fig. 4: Observed and predictive nitrate concentration under 0.50 m water table treatment

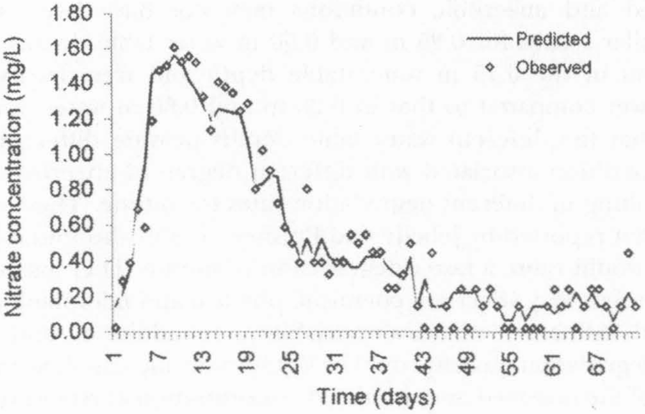

Fig. 5: Observed and predictive nitrate concentration under 0.75 m water table treatment

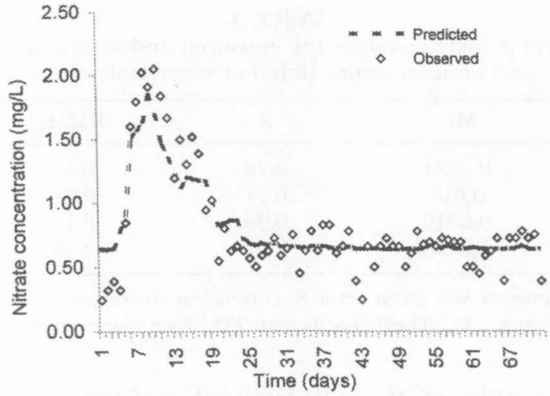

Fig. 6: Observed and predictive nitrate concentration under free water table treatment

model prediction match the observed data. Statistical methods suggested by Voltz and Webster (1990) was used to evaluate the simulation capability of the model. The statistical parameters used in this study are: the mean error (ME). This quantity measures the bias of the prediction and should be close to zero for unbiased methods. The second parameter is the root mean square error (RMSE) that measures the absolute size of the error. This measure is similar to the mean absolute error except that the squaring function is used instead of the absolute value function. It is more sensitive to large errors than the mean absolute error. Furthermore, the regression model was also tested using Theil's coefficient U that is given by Naylor (1970). The mathematical expressions of these statistical parameters are as described below.

$$ME = 1/n \quad (P_i - A_i) \tag{2}$$

$$RMSE = \quad 1/n \quad (P_i - A_i)^2 \tag{3}$$

$$U = \frac{\sqrt{\frac{1}{n} \quad (P_i - A_i)^2}}{\sqrt{\frac{1}{n} \quad P_i^2} + \sqrt{\frac{1}{n} \quad A_i^2}} \tag{4}$$

where n is the number of samples, P_i is the observed value and A_i the simulated one.

The values obtained for each statistical parameter under different water table depths are listed in Table 3. The calculated mean error values between measured and simulated in all water table depths was close to zero. Also low values of root mean square error were observed in all water table depths. A high value of correlation coefficient between measured and simulated data was observed for all water table depths. Beside these, the values of Thiel's coefficient was calculated in all water table depths According to the limits of the numerical

TABLE 3
Statistical parameter values for measured and simulated nitrate concentration under different water table depths

WT	ME	R	RMSE	U
0.25m	-0.0034	0.78	0.17	0.20
0.50m	-0.017	0.71	0.24	0.23
0.75m	-0.0019	0.96	0.12	0.86
FD	-0.0098	0.92	0.18	0.019

W T: water table treatments ME: mean error R: correlation coefficient
R: Root-mean-square error U : Theil's coefficient FD : Free water table.

values of Thiel's coefficient, the calculated value of this coefficient was found close to zero, which indicates perfect agreement between the model predictions and observed data in all water table depths. These statistics demonstrate good agreement between simulated and measured data under different water table depths.

CONCLUSIONS

Several conclusions can be drawn from this study. The water table depth is an important factor affecting nitrate transport. The degree and extent of saturation in the soil profile as a result of different water table depths may enhance the biological and chemical degradation of the contaminants such as fertilizer and herbicides. Under water-saturated conditions, denitrification capacity could be significantly increased and low concentrations of nitrate were observed. A suitable soil water condition may maintain a soil-water microenvironment at a favorable level, which would enhance some soil chemical, physical and microbiological activities. These activities can breakdown the contaminants and cause less risk of pollution to the water systems. Based on the experimental results, a simple statistical model was developed to simulate the reduction in nitrate transport under different water table depths. For all water table treatments, the model simulations are not significantly different from the observed data. The statistical parameters that included mean error, root mean square error, correlation coefficient, determinations coefficient R^2 and Theil's coefficient were used to test the simulation capability of the proposal model under different water table treatments. The parameters demonstrate good agreement between model simulation and measured data under different water table depths.

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