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STRUCTURAL EQUATION MODELING OF DYNAMICS OF NITRATE CONTAMINATION IN GROUND WATER[1]

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ABSTRACT: Most research on the temporal aspect of nitrate pollution in water resources has focused on surface water. Comprehensive studies on the dynamics of nitrate in ground water are lacking, especially on a drainage basin scale and for relatively long periods of time. In this study, structural equation modeling is applied in investigating the influences of climate, hydrology, and nitrogen management in agricultural production on nitrate concentration in the Big Spring Basin, Iowa, over a 10-year period. The study shows that for given hydrogeological settings, nitrogen management practices and climate are the two most important factors that affect nitrate dynamics. The long-term trend of nitrate is closely related to the nitrogen input primarily determined by management practices. The potential effects of nitrogen management, however, are contingent on the variations of climate. The improvements in water quality (reduced nitrate concentration and loads) in relation to improved nitrogen management are often overshadowed by the impact of climate, especially in extremely dry or wet years. The variations of climate and hydrology have much greater impacts on the nitrate dynamics than the changes in nitrogen input. This study reveals significant seasonal variation in the relations between nitrate concentration and influencing factors, which is also closely related to the seasonal variation in climate. Assessment of management practices and resultant water quality should consider the impact of short- and long-term climate dynamics.
(KEY TERMS: structural equation modeling; nitrate dynamics; ground water; non-point source pollution; agriculture.)

INTRODUCTION

Agriculture is generally recognized as the leading nonpoint source of water pollutants, such as sediments, nutrients, and pesticides (National Research Council, 1989, 1993). Among other water pollution problems related to agriculture, nitrate pollution has been of growing concern. Nitrate contamination from agricultural activities has been reported in almost every state in the United States (Madison and Brunett, 1985; Hallberg, 1989). High nitrate loads have continued, or increased in many streams in the country, despite the reduction in point source contributions as a result of implementation of the Clean Water Act passed in 1972 (Smith *et al.*, 1987). A survey conducted in Iowa in 1988-1989 showed that for private domestic water supply (DWS) wells that are less than 15 meters deep, 35 percent of sampled wells exceeded 10 mg/L NO_3-N, the maximum contamination level (MCL) set by the U.S. Environmental Protection Agency (USEPA). In some counties in Iowa, approximately 70 percent of DWS wells exceeded the MCL (Hallberg *et al.*, 1990; Kross *et al.*, 1990).

Nitrate pollution has come under increasing study for the past two decades (Commoner, 1972, 1977; Hill, 1978; Aldrich, 1980; Follett, 1989; Hallberg and Keeney, 1993). Many of the studies have been short-term, or event-oriented. Studies on the temporal change, or dynamics of nitrate in water resources have focused on surface water, especially streams or rivers. The effects of influencing factors are often investigated in isolation. Long-term comprehensive studies on nitrate contamination in ground water are lacking, especially those on a drainage basin scale.

This study investigates the dynamics of nitrate in the ground water in the Big Spring Basin in Iowa, during a span of ten years, from water year 1982 through water year 1991. The influences of climate, hydrology, and nitrogen management are examined at the basin, or watershed scale, using structural equation modeling techniques.

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Big Spring Basin Project

Extensive studies in the Big Spring ground water basin in northeastern Iowa (Figure 1) have been significant in defining agricultural nonpoint source impacts on water quality. Historic data illustrated that regional increases in nitrate in ground water paralleled increasing fertilizer-nitrogen rates and corn acreage since the 1960s (National Research Council, 1993; Hallberg and Keeney, 1993). The hydrology, water quality, agricultural, and land-use practices in the Big Spring Basin have been studied since 1981 (e.g., Hallberg *et al.*, 1983; Libra *et al.*, 1992; Rowden *et al.*, 1995a). The land in the 267 km^2 basin is essentially all used for agriculture. There are no significant urban or industrial areas, no landfills, or other major point sources that may affect groundwater quality (Hallberg *et al.*, 1983).

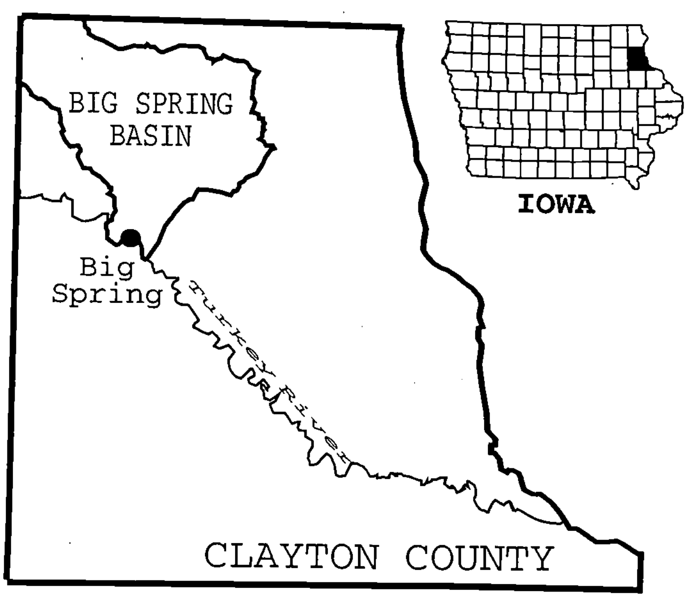


Figure 1. Location of the Big Spring Basin.

The basin is named after Big Spring, the largest ground water spring in Iowa, which discharges from the underlying Galena aquifer, a group of Ordovician-age carbonate rock units. The Galena aquifer is unconfined over most of the basin area and is mantled by 1-15 meters of loess and glacial drift. The combination of agroecosystems and a responsive hydrogeological system in the basin offers a good setting for studying the impact of non-point source pollution by agriculture on groundwater quality (Libra *et al.*, 1992). The research and monitoring activities in the basin provide long-term data for quantifying water quality and its variation over time in relation to management practices in agricultural production.

Big Spring is the principal discharge point for the ground water basin. Extensive past studies on the hydrogeology indicate that the outflow from Big Spring comprises approximately 90 percent of the ground water discharge from the basin (Hallberg *et al.*, 1983; Littke and Hallberg, 1991). The spring has been instrumented to continuously measure its discharge. The ground water discharging from the spring integrates the water quality from the whole basin. The nitrate concentration at the spring is very close to the averages (mean and median) of the values from extensive well inventories in the basin (Hallberg *et al.*, 1983; Hallberg, 1987; Liu *et al.*, 1997). The dynamics of nitrate discharging at the spring can be considered representative of the basin as a whole (Hallberg *et al.*, 1993).

In addition, a major technology transfer effort to improve farm management, the Big Spring Basin Demonstration Project (BSBDP), was initiated in the basin by a multi-agency group. Field leadership was provided by Iowa State University (ISU) Extension; improvements in nitrogen management were particularly targeted. Through the BSBDP, basin farmers have reduced fertilizer-N rates for corn by about 30 percent since the early 1980s with no yield loss, reducing environmental loading and providing enhanced profitability for area farmers (Hallberg, 1996).

The significant, but gradual, incremental changes in N-management in the basin would take time for definitive assessment of related water-quality improvements at the basin scale, even under the best of circumstances. Assessment of possible water-quality improvements has been confounded by the climatic aberrations of recent years (Hallberg *et al.*, 1993; Rowden *et al.*, 1995b). In this paper, structural equation modeling is used as a tool to further understand the dynamics of nitrate, water quality, climate, and land management in the basin.

Structural Equation Modeling of Time Series

When data are collected in an ordered sequence at equally spaced intervals over time, they are usually called time series. Analysis of this kind of data is usually called time series analysis. In a narrow sense, time series analysis usually refers to the time series model approach associated with the work of Box and Jenkins (1976). Time series modeling of the Box-Jenkins type involves fitting models to one or more time series that describe the system under study for the purpose of analyzing, interpreting, or forecasting. The time series modeling approach introduces the concepts and techniques for dynamic modeling (Harvey, 1990). The weakness of the Box-Jenkins approach to modeling time series lies in its exploratory nature. It is an empirically-based and data-driven approach. The structure of a time series model is derived from the observed data instead of from theory (Ostrom, 1990).

In contrast, a theory-driven approach to time series modeling is based on logic, theory, and knowledge of the system under study. In a structural equation model, the model structure is posited first on the basis of relations by theory. The model is then tested with the data to determine whether there exists empirical support for the specified structure (Saris and Stronkhorst, 1984; Hayduk, 1987). Because of its theory-driven nature, structural equation models have been widely used in causal modeling for non-experimental studies, especially in some social sciences, such as sociology, economics, and psychology (Blalock, 1971; Duncan, 1975; Joreskog, 1977; Harvey, 1990). This approach has also been applied in natural sciences, especially in recent years (Westman, 1978; Malanson and Trabaud, 1988; Johnson *et al.,* 1991; Rhoads, 1992).

In applications of structural equation modeling, the specification of causal proposition is not based on the statistics, not even on the data (although the availability of data must be taken into account). It is the investigator's responsibility to specify the model structure in causal modeling, while the role of the observed data and statistical procedures is to detect the defects in the specifications. Data analysis with structural equation modeling may result in rejecting the proposed putative causal structure, or it may fail to do so. This is the most critical difference between structural equation modeling and the Box-Jenkins approach in time series analysis. That is, it is confirmatory versus exploratory.

One should keep it in mind that there are different opinions with regard to whether observational (non-experimental) data can be used for searching causal relations (Saris and Stronkhorst, 1984). The same is true of whether the structural equation modeling approach is more theory-driven than other approaches, such as Box-Jenkins methods in time series analysis. We believe that the debate is more philosophical than technical. On one hand, there is no statistical procedure that automatically leads to a revelation of causal relations from observational data. This is also the case with structural equation models. On the other hand, the structural equation modeling approach does allow one to specify likely causal relations based on theories and knowledge of the system under study, and then use the data to test for validity of the specification.

Technically speaking, structural equation modeling is an extension of regression technique. A regression model can be considered as a special case of structural equation models. However, more complicated relations can not be specified using regression models, such as a recursive set of equations (as applied in this study), and interdependence or simultaneous systems (Joreskog and Sorbom, 1989).

A structural equation model consists of a system of equations. Each equation in the model represents possible causal links between an endogenous variable and other endogenous variables as well as exogenous variables. The structural form of the model can be regarded as a theoretical explanation or hypothesis about the determination of endogenous variables.

Endogenous variables are those determined by the system. They are also called jointly dependent variables, or response variables. Endogenous variables are influenced by other endogenous variables and/or exogenous variables, either directly or indirectly. The variation in the values of endogenous variables is to be explained by the model. These variables appear on the left-hand side as well as on the right-hand side of equations.

Exogenous variables are those determined outside the system. They are predetermined or independent variables. The variation in the values of exogenous variables is not to be explained by the model. These variables always act as causes and never as effects. Correspondingly, they only appear on the right-hand side of equations.

METHODS

Data used in this study include: nitrate-N concentration data from Big Spring; ground water and nitrate-N discharge from the spring; nitrate-N discharged in surface water from the basin; air temperature, precipitation, potential evapotranspiration (PET) for the basin; and a nitrogen balance for the basin. All the data used are monthly averages. The total number of observations for ten years is 120.

The water-quality, discharge, and precipitation data for the basin were derived from various summary reports from the monitoring and gauging efforts in the Big Spring basin, conducted by the Iowa Department of Natural Resources, Geological Survey Bureau, and USGS (e.g., Rowden *et al.,* 1993, 1995b). Air temperature was derived from reports of the National Oceanic and Atmospheric Administration (NOAA). PET was estimated using the Blaney-Criddle Formula (Dunne and Leopold, 1978). Data for the nitrogen balance were derived from crop and livestock inventories in the basin, including fertilization rates, using standard assumptions for nitrogen availability from manure and alfalfa, and monthly and annual crop uptake estimates developed by ISU Extension (Hallberg, 1987; National Research Council, 1993; Liu, 1995).

Nitrate concentration in water samples was analyzed by the University Hygienic Laboratory (UHL) in Iowa City, a U.S. Environmental Protection Agency certified laboratory. The nitrate data are presented in this paper as NO_3-N unless otherwise indicated.

The search for potential causal structure for observed nitrate dynamics at the scale of the Big Spring basin falls within the framework of causal modeling in non-experimental research. As such, structural equation models are applied to the analysis of nitrate dynamics. In this study, nitrate concentration and ground water discharge at Big Spring are chosen as endogenous variables. For the completeness of the equation system, two equations are specified. Exogenous variables in the equations include precipitation, air temperature, potential evapotranspiration, and nitrogen balance. The data for nitrate and other variables are time series data and the structural equation model is solved at each point in time. As such, the model is considered as a discrete-time dynamic model.

Since nitrate concentration is affected by discharge, but not vice versa, the structural equation model for this study will take the form of a recursive system as shown in the following:

$$QT_t = \gamma_{11}P_t + \gamma_{12}PET_t + u_{1t} \qquad (1)$$

$$NO_3N_t = \beta_{21}QT_t + \gamma_{23}T_t + \gamma_{24}N_t + u_{2t} \qquad (2)$$

where t is time point (month), t=1,2, . . . , 120; γ_{11}, γ_{12}, γ_{23}, γ_{24}, and β_{21} are coefficients; NO_3N is nitrate concentration as NO_3-N at Big Spring; QT is water discharge from the spring; P is precipitation; PET is potential evapotranspiration; T is air temperature; N is nitrogen balance in the basin; u_{1t} and u_{2t} are error terms.

The same relations specified by the model can also be represented by a path diagram as shown in Figure 2.

Evapotranspiration (ET) is a major component of the water cycle and water balance. Besides precipitation, ET is another climatic factor that plays an important role in controlling water recharge to ground water. When data on ET are not available, potential evapotranspiration (PET) can be used as a substitute. That is why PET is included in Equation (1) for water discharge (QT). Monthly mean air temperature and monthly day-time hours as a fraction of yearly day-time hours are the driving factors in the Blaney-Criddle Formula for estimating PET. In addition, effects of crop cover are also considered in the formula (Dunne and Leopold, 1978, pp. 139-141). Air temperature is included in Equation (2) for nitrate concentration because of its influence on soil temperature, biotic activities, mineralization, and other processes in the nitrogen cycle

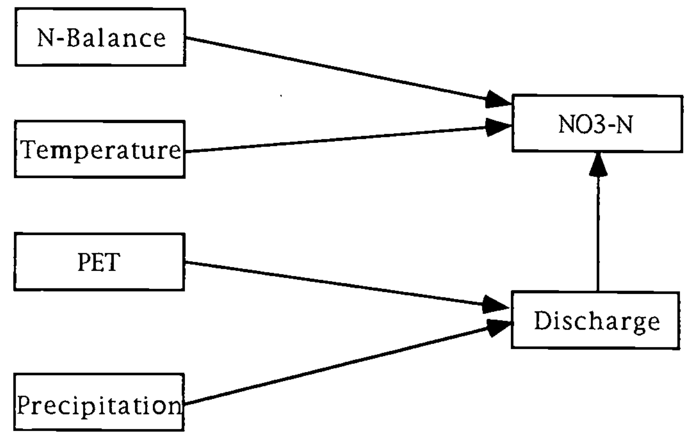


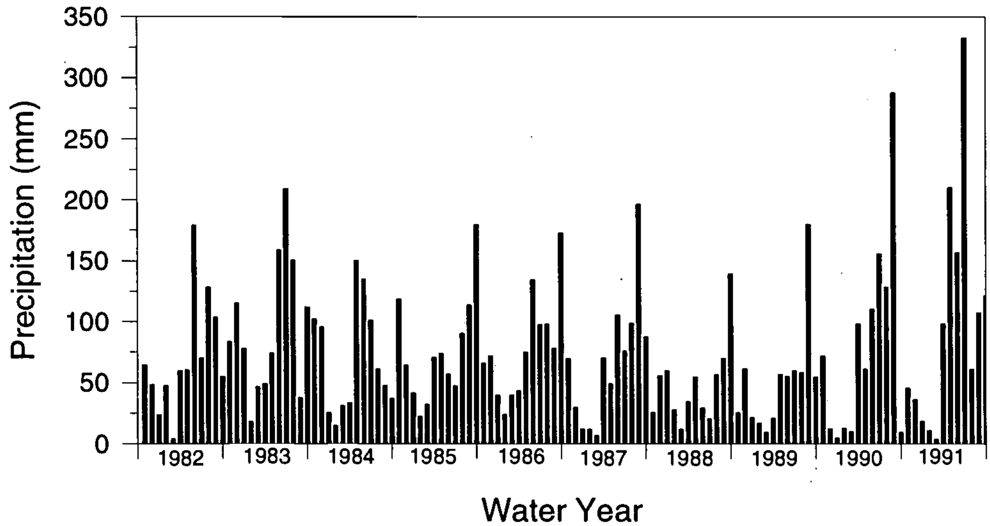
Figure 2. A Simplified Path Diagram for the Relations Specified in the Structural Equation Model (Equations 1 and 2).

ANALYSES AND RESULTS

Figure 3 shows plots of the monthly precipitation in the basin and deviations from the norms of the study period (WYs 1982-1991). Figures 4 and 5 show the ground water discharge and nitrate concentration at the spring. In Table 1, the average monthly values over the study period (10 years) are given for precipitation, discharge, PET, net nitrogen input, and nitrate concentration; the annual averages are listed in Table 2.

Both extreme drought and wet conditions were observed during the period of study. The drought in WYs 1988 and 1989 is indicated by the lowest values of annual precipitation (582.8 mm and 617.9 mm). The flooding in WY 1991 is revealed by the highest precipitation of the decade (1201.1 mm) (Table 2 and Figure 3). The impact of both lack and excess of precipitation was prominent. The drought led to the lowest values in both water discharge and nitrate concentration in 1989, while the excess precipitation resulted in the highest values in 1991 (Table 2, Figures 4 and 5).

The impact of nitrogen input on nitrate concentration was overshadowed by extreme conditions of precipitation. This was most obvious in 1991 when the



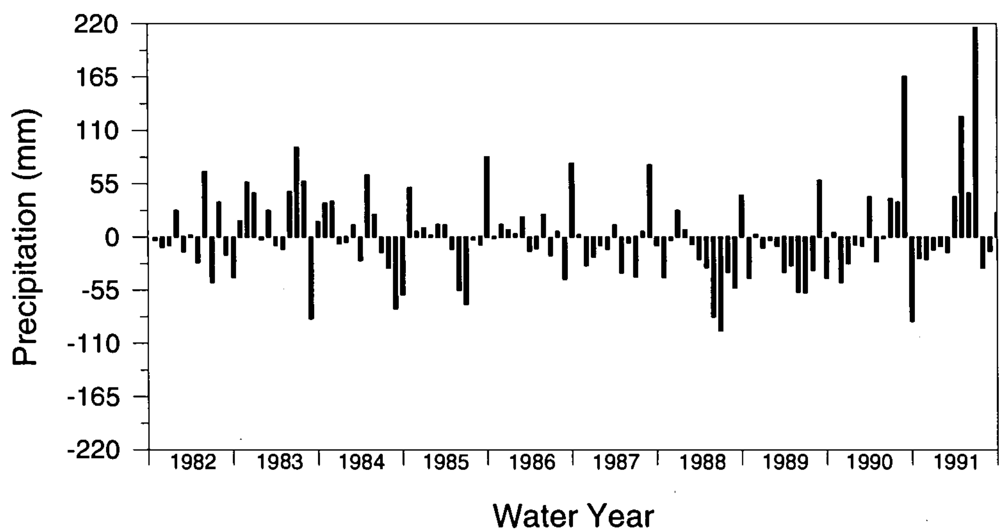


Figure 3. Monthly Precipitation in the Basin (above) and Its Deviation from the Norm of the Period from WYs 1982 to 1991 (below).

record-high nitrate concentration was observed despite the low nitrogen input in that year and a number of previous years.

Nitrogen Balance in the Basin

A partial nitrogen budget is used in this study. That is, only those major sources or sinks of nitrogen that are manageable in the process of agricultural production are included in the nitrogen budget (National Research Council, 1993). The major inputs considered include nitrogen in commercial fertilizer, the available nitrogen in manure, and nitrogen fixed by legumes (alfalfa) and available to a subsequent crop. The major output is nitrogen uptake by crops and removal in the harvest. The result of the nitrogen budget is the net nitrogen input from a management practice point of view:

$$\text{Net N input} = \text{N in fertilizer} + \text{N in manure} + \text{N fixed by legumes} - \text{N in harvest}$$

While there are other input sources, such as nitrogen deposition from precipitation, these considered

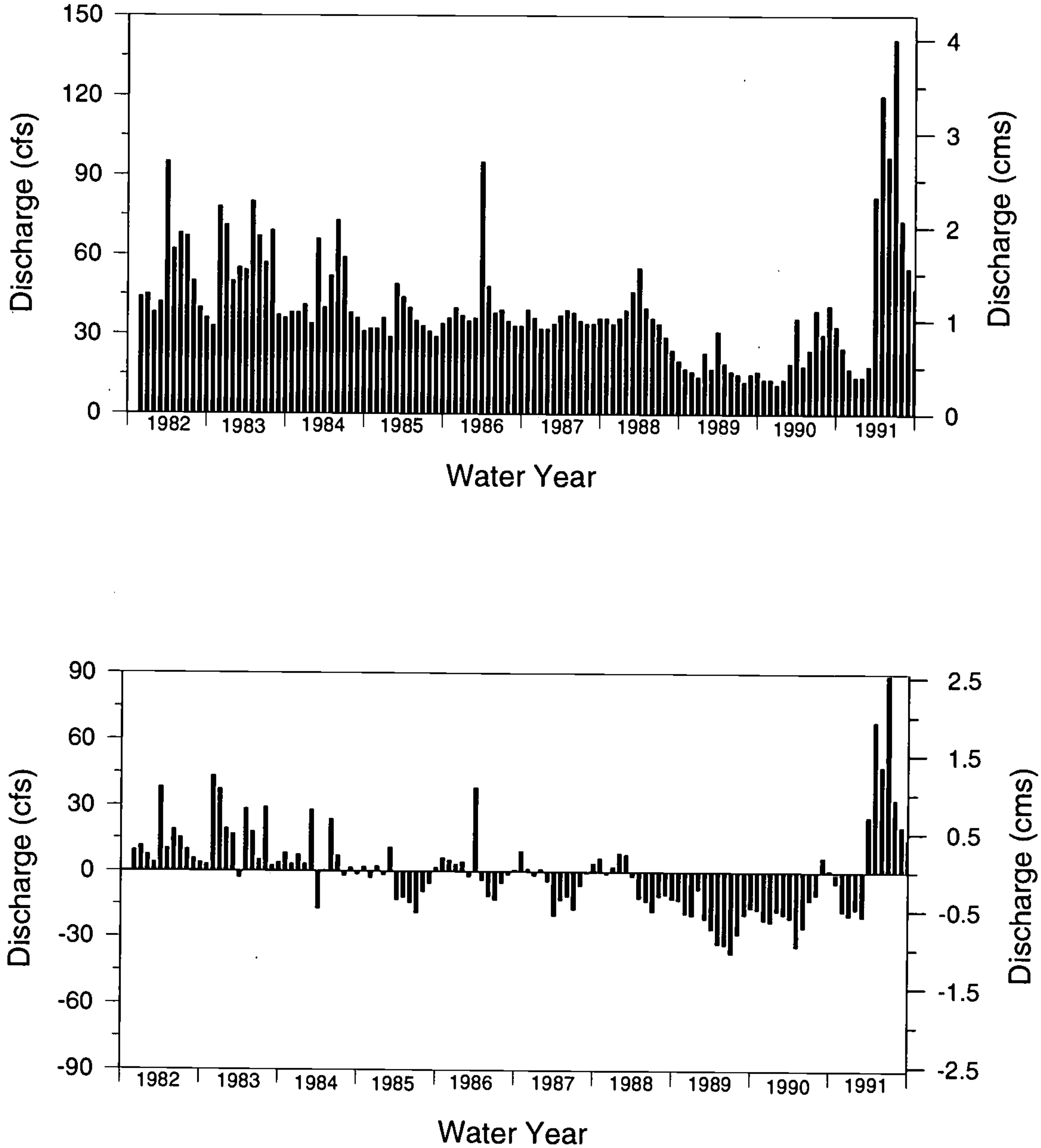


Figure 4. Monthly Water Discharge From Big Spring (above) and Its Deviation from the Norm of the Period from WYs 1982 to 1991 (below).

here are the greatest and constitute approximately 85-90 percent of the annual nitrogen inputs (Hallberg, 1987).

Nitrogen losses in forms other than harvesting, such as denitrification in the soil and other gaseous losses (e.g., ammonia volatilization), are other important nitrogen sinks. One important component of gaseous losses has already been taken into account when nitrogen losses are factored into the estimate of nitrogen available from manure. However, there is no reliable way to estimate other gaseous losses from the soil on a basin scale; hence, these losses were left out of the budget equation.

Estimates of denitrification and gaseous losses from the soil excluded from the nitrogen budget are usually small relative to other pathways, such as harvesting and loss to water systems. Some upper estimates can reasonably reach an equivalent of 20 percent of the fertilizer nitrogen applied (NRC, 1993). If this upper end estimate is used, the value derived is less than the estimated nitrogen input from precipitation, which was also left out of the budget equation. In short, those nitrogen inputs and gaseous losses not included in the nitrogen balance can be considered, to some extent, to cancel out

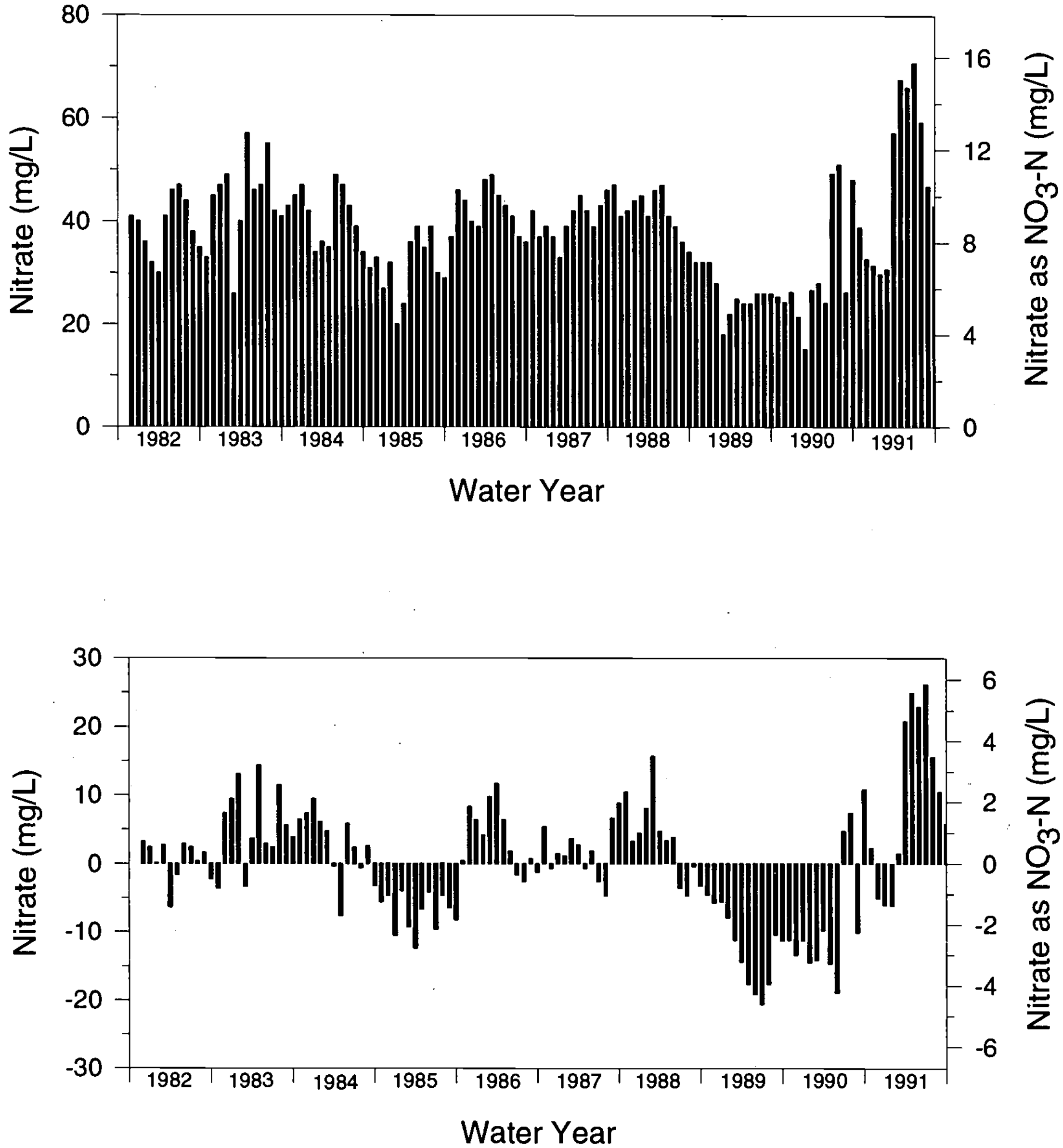


Figure 5. Monthly Nitrate Concentration at Big Spring (above) and Its Deviation from the Norm of the Period from WYs 1982 to 1991 (below).

It is practically impossible to accurately describe the nitrogen storage in the basin at any given time. The data on the net nitrogen input and losses in forms other than harvesting make it possible to assess the changes in nitrogen storage in the basin since the beginning of the study period. If there were no other losses, the cumulative sum of the net nitrogen input from management was equivalent to the change in nitrogen storage in the basin from the starting point (October, 1981) to any point of interest in time.

Table 3 lists the net nitrogen input for each water year of the study period. In each year, the input of nitrogen exceeded the need of crop plants for nitrogen (shown as N_Input in Table 3) and a large amount of excess nitrogen accumulated in the basin. The ten-year total of excess nitrogen input is 9,947 Mg. In other words, the nitrogen storage in the basin would have increased by almost 10,000 Mg if no other losses occurred during the same period of time.

A substantial mass of nitrogen is removed from the basin in ground water and surface water discharge. To account for loss of nitrogen from the basin in ground water and surface water, Big Spring and Roberts Creek were considered. The former discharges from the underlying aquifer and the latter

TABLE 1. Monthly Averages for Precipitation (P), Discharge (QT), Potential Evapotranspiration (PET), Net Nitrogen Input (N-Input), and Nitrate Concentration in Ground Water (as NO_3-N), for WYs 1982-1991.

Month	P (mm)	QT (cms)	PET (mm)	N-Input (Mg)	NO_3-N (mg/L)
January	20.6	0.87	4.7	0	8.0
February	19.6	1.08	6.4	0	6.5
March	57.7	1.61	14.8	24	8.1
April	86.3	1.47	37.5	1,011	9.5
May	111.9	1.39	79.0	957	9.6
June	116.8	1.47	142.0	-87	9.9
July	93.0	1.14	191.9	-902	9.7
August	122.2	0.97	150.9	-323	8.1
September	96.7	0.91	65.0	60	8.3
October	67.5	0.85	32.8	158	8.1
November	58.9	0.99	11.7	116	8.4
December	32.3	0.95	6.2	0	8.4

TABLE 2. Annual Averages or Sums for Precipitation (P), Water Discharge (QT), Potential Evapotranspiration (PET), Net Nitrogen Input (N-Input), and Nitrate Concentration (NO_3-N).

WY	P (mm)	QT (cms)	PET (mm)	N-Input (Mg)	NO_3-N (mg/L)
1982	849.6	1.51	676.3	1,382	8.7
1983	1,131.0	1.62	733.9	1,703	9.8
1984	833.4	1.29	692.5	1,470	9.2
1985	910.4	1.00	707.0	1,157	6.9
1986	938.8	1.19	751.7	736	9.4
1987	812.3	1.01	820.1	799	9.0
1988	582.8	1.01	817.9	1,549	9.3
1989	617.9	0.50	708.5	446	5.8
1990	961.9	0.68	742.0	302	6.8
1991	1,201.1	1.66	779.8	403	10.6

TABLE 3. Net Nitrogen Input From Management Practices (N_Input), Nitrogen Losses at Big Spring (N_BSP) and at the Outlet of Roberts Creek (N_RC), Difference Between Input and Losses (N_B), and Cumulative Difference (C_N_B) at End of Each Water Year (Unit: Mg).

WY	N_Input	N_BSP	N_RC	N_B	C_N_B
1982	1,382	378	194	810	810
1983	1,703	522	254	927	1,737
1984	1,470	382	144	94	2,681
1985	1,157	215	31	911	3,592
1986	736	358	100	278	3,870
1987	799	283	106	408	4,278
1988	1,549	304	87	1,158	5,436
1989	446	89	8	349	5,785
1990	302	176	50	76	5,861
1991	403	656	468	–721	5,140

accounts for over 70 percent of the surface water flow leaving the basin. The annual losses of nitrogen from Big Spring and from the monitoring site at the Roberts Creek are also given in Table 3 (N_BSP and N_RC), along with the difference between net input from the management and the combined losses at these two sites (N_B), and the cumulative nitrogen balance at end of each water year (C_N_B).

The nitrogen loss in surface water in Roberts Creek does not account for all the nitrogen loss in the surface water system in the basin. One reason is that Roberts Creek is not the only stream discharging from the basin. Also in-stream processes reduce the nitrate load in streams, especially in summer, through denitrification and consumption by aquatic biota (Hill, 1983; Bachman *et al.*, 1991). These may also be part, though not a large part, of the large difference observed between net nitrogen input from the management and nitrogen losses at these two sites.

Denitrification in the soil and other gaseous losses also account for part of this difference. The values of N_B and C_N_B in Table 3 would be reduced if those nitrogen losses were accounted for.

Ground water, through discharge at Big Spring, is the dominant sink of nitrogen residues in the basin. Nitrogen loss from the basin through surface water (Roberts Creek) was only about half of the loss at Big Spring at the end of the first year (WY 1982). The ratio between the two then consistently declined each year and reached as low as 36 percent at the end of WY 1990. Then it climbed up to 43 percent in WY 1991, with greatly increased surface water discharge in the wettest year during the study period.

Although it is practically impossible to estimate all the nitrogen losses to surface and groundwater systems, the two sites considered are the two major dominant sinks that accounted for a great portion of nitrogen loss to the water systems in the basin. On the other hand the amount of nitrogen removed from the basin through these two sites only made up 48 percent of the net nitrogen input during the decade. The nitrogen residues in the basin continued to increase each year (shown as C_N_B in Table 3) until the last year of the study period, WY 1991. In that year, excess precipitation generated flooding in the area and also caused tremendous loss of nitrogen related to the large discharge of water. Nitrogen loss reached the decade's highest level at both Big Spring and Roberts Creek in 1991. As a result, the first decline in the basin's nitrogen storage in the decade was observed. That, however, was an exception to the changes in nitrogen storage in the basin. The deficit in nitrogen balance in water year 1991 (-721 Mg; Table 3 and Figure 6) was also an indication of the large nitrogen storage in the basin that exists as a result of excess nitrogen inputs in previous years. Although some nitrogen losses, such as denitrification and other gaseous losses, were uncounted for, these

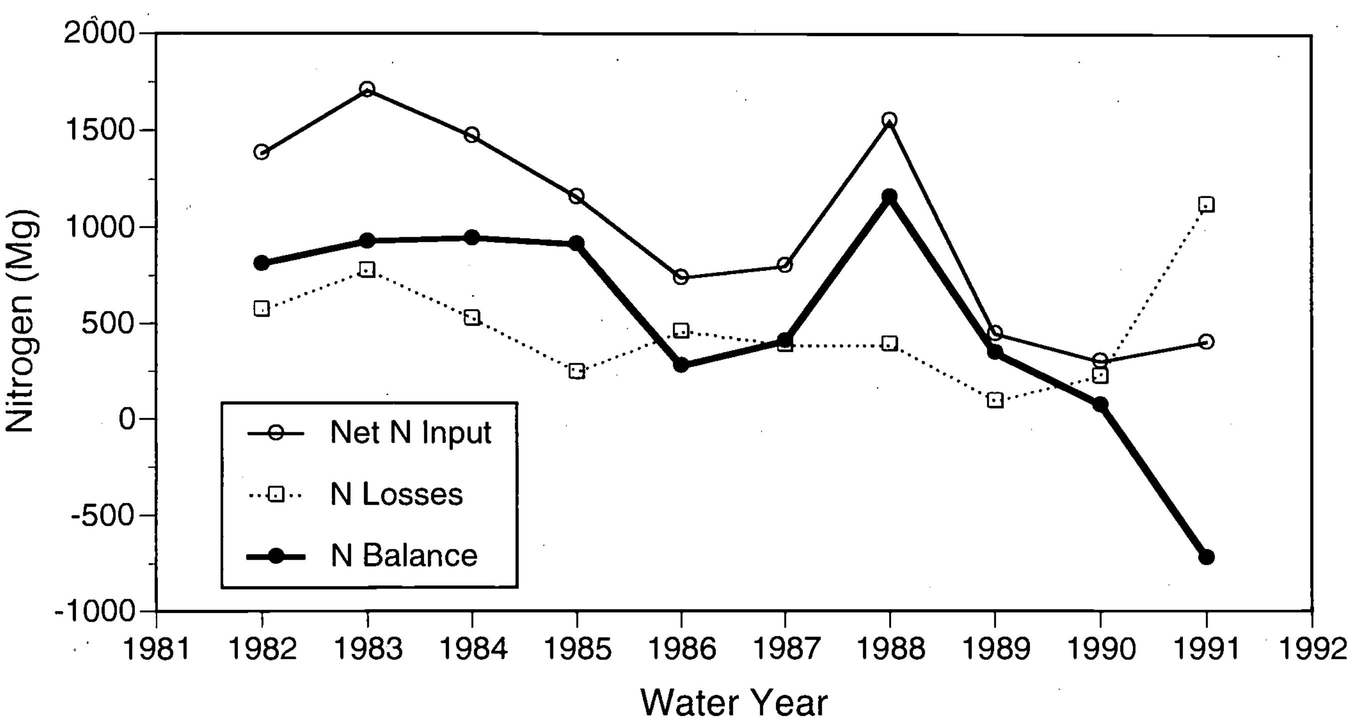


Figure 6. Annual Changes in Net Nitrogen Input From Agricultural Production, Nitrogen Losses to the Ground and Surface Water Systems, and Nitrogen Balance (difference between input and loss) in the Big Spring Basin.

losses and those nitrogen inputs excluded from the nitrogen balance (such as wet nitrogen deposition) would cancel out to some extent. Therefore, it is reasonable to conclude that even if all the sinks of nitrogen were counted, a large portion of net nitrogen input from farming operations still would be retained in the basin.

Changes in nitrogen management and nitrogen balance in the basin can be measured in two ways, i.e., monthly nitrogen balance, defined as the difference between input and output, and the cumulative change in nitrogen storage in the basin. The cumulative change was used in the study because with regard to nitrate dynamics, what counts is the amount of nitrate available for leaching to the ground water. That is, even when a particular monthly nitrogen balance is small or in deficit, the nitrate concentration may still remain high as long as there is nitrogen in storage that can be mobilized. Although it is impractical to specify the total nitrogen storage in the basin that would contribute to the leaching process, the estimated cumulative change in the nitrogen storage can be used to assess the relation between change in nitrogen management and nitrate dynamics.

One missing piece is the value of nitrogen storage at the beginning of the study period. If we assume that the value was "S," the nitrogen storage at any time since then would be S plus the cumulative change in nitrogen storage. Adding the constant S to all the values of cumulative change in nitrogen storage will not make any difference with regard to modeling its relation with nitrate concentration in the ground water. This provides a way to avoid the difficulty in estimating the total nitrogen storage in the basin while still being able to investigate the role of nitrogen management in nitrate dynamics.

Structural Equation Modeling

Based on logic, theory, and knowledge of the basin, causal orders of the six variables used in the modeling process were determined and causal hypotheses were specified:

1. The temporal variation in discharge is primarily controlled by climatic variation. Two factors of climate, precipitation and potential evapotranspiration, determine the amount of water recharged to the aquifer, therefore exerting direct impact on the discharge at the outlet of the aquifer.

2. Since nitrate leaching is associated with the recharge process, high discharge is generally accompanied by high nitrate concentration. Thus, discharge, which provides an integrated measure of hydrological conditions in the basin, has a direct relation to nitrate concentration.

3. Through discharge, most climate factors indirectly affect nitrate concentration.

4. Air temperature exerts a direct impact on nitrate dynamics by affecting soil temperature, biotic activities, mineralization and other processes in the nitrogen cycle.

5. Cumulative change in nitrogen storage in the basin has direct influence on nitrate concentration by controlling the amount of nitrogen available for nitrification and leaching to the ground water.

These hypotheses constitute the structural equation model given in Equations (1) and (2), and Figure 2.

NO_3-N (NO_3N) and QT are endogenous variables and determined by the equation system. The variation in the observed values of NO_3-N and QT is to be explained by the model. The other variables are exogenous variables and determined outside the system. The variation in the values of those variables is not to be explained by the model. As shown in the model, NO_3-N is influenced by another endogenous variable, QT, and some exogenous variables. QT is influenced only by exogenous variables.

Some modifications were made to the above model based on the following considerations. A time lag exists between nitrate leaching in the basin and its appearance at the basin outlet. As such, air temperature (T) and cumulative change in nitrogen storage (N) that have direct impact on nitrate leaching were lagged by one time unit (one month).

The current status of a hydrological system is often influenced by the system's antecedent conditions. In most practical problems, the influence is primarily from the most recent past, or one lagged time unit. In this study, the rate of water discharge in the current month is partly dependent on the water discharge a month before. Likewise, the nitrate concentration in the current month in part depends on the nitrate concentration in the previous month. Statistically, this phenomenon is generally reflected as correlations (autocorrelation) between temporally adjacent observations of the same variable. This autocorrelation structure can be described by a first-order autoregressive process, or AR(1). The AR(1) process can be incorporated into the model by including a time lag of one time unit, i.e. one month in this study. Because of the responsiveness of the hydrogeological system in the basin, the influence beyond one month is negligible. To account for the influence of antecedent conditions, lagged QT and NO_3-N by one time unit (a month) were included in the model as extra exogenous variables. The modified model is given in the following:

$$QT_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*QT_{t-1} + u_{1t} \quad (3)$$

$$NO_3N_t = \alpha_2 + \beta_{21}*QT_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*NO_3N_{t-1} + u_{2t} \quad (4)$$

where t is time point (month), t =1,2, . . . ,120; α_1, α_2, γ_{11}, γ_{12}, γ_{13}, γ_{24}, γ_{25}, γ_{26}, and β_{21} are coefficients; NO_3N is nitrate concentration as NO_3-N at Big Spring (mg/L); QT is water discharge from the spring (cms); P is precipitation (mm); PET is potential evapotranspiration (mm); T is air temperature (Celsius); N is cumulative change in nitrogen storage in the basin (Mg); u_{1t} and u_{2t} are error terms with zero means and a multivariate normal distribution.

The model can also be expressed in matrix form:

$$\mathbf{Y_t} = \mathbf{A} + \mathbf{B}^*\mathbf{Y_t} + \Gamma^*\mathbf{X_t} + \mathbf{u_t}, \qquad t=1,\ldots 120 \quad (5)$$

where

$\mathbf{Y_t} = [QT_t, NO_3N_t]'$;

$\mathbf{X_t} = [P_t, PET_t, QT_{t-1}, T_{t-1}, N_{t-1}, NO_3N_{t-1}]'$;

$\mathbf{A} = [\alpha_1, \alpha_2]'$;

$$\mathbf{B} = \begin{bmatrix} 0 & 0 \\ \beta_{21} & 0 \end{bmatrix};$$

$$\Gamma = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} & 0 & 0 & 0 \\ 0 & 0 & 0 & \gamma_{24} & \gamma_{25} & \gamma_{26} \end{bmatrix};$$

$\mathbf{u_t} = [u_{1t}, u_{2t}]'$; and

$\mathbf{u_t}$ is assumed to have mean zero and a multivariate normal distribution.

The SAS procedure PROC SYSLIN (SAS, 1988) was applied in the structural equation modeling. The residual plots from fitting the model in (5) revealed non-constant variance in QT and NO_3-N. Log transformation was then performed on the original observations of these two variables. The results from fitting the model to the transformed data are given in Table 4.

As indicated by t-values and p-values in the table, both precipitation (P) and potential evapotranspiration (PET) showed significant impact on water discharge. The two are different, however, in that the former has a positive and the latter has a negative relation with discharge. That is, an increase (or decrease) in precipitation will result in a corresponding increase (or decrease) in discharge; while an increase (or decrease) in PET will lead to a decrease (or increase) in discharge. Also, the magnitude of discharge of the previous month has a significant and positive impact on the discharge in the current month, showing the influence of antecedent conditions on hydrologic responses.

All factors in the second equation showed significant and positive effects on nitrate concentration, increases in air temperature, water discharge, and/or nitrate storage will cause nitrate concentration to increase. Also, the nitrate concentration of the previous month positively affects the current month's

TABLE 4. Results From Structural Equation Modeling (whole year).

$LOG(QT)_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*LOG(QT)_{t-1} + u_{1t}$

Variable	Parameter Estimate	T-Value	P-Value
P	0.0023	4.55	0.0001
PET	-0.0018	-4.06	0.0001
LAG(LOG(QT))	0.7741	14.72	0.0001

$LOG(NO_3N)_t = \alpha_2 + \beta_{21}*LOG(QT)_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*LOG(NO_3N)_{t-1} + u_{2t}$

Variable	Parameter Estimate	T-Value	P-Value
LOG(QT)	0.32950	6.61	0.0001
LAG(T)	0.00308	2.17	0.0318
LAG(N)	0.00002	2.32	0.0223
LAG(LOG(NO3N))	0.37296	5.16	0.0001

Notes: 1. Parameter estimates are those of full information maximum likelihood.
2. R-squares are 0.71 and 0.65 for Equations 1 and 2, respectively.
3. R-square for the equation system is 0.67.

nitrate concentration, showing the influence of antecedent conditions.

As a result of log-transformation, the estimated parameter values given in Table 4 do not have the usual interpretation that the value of a parameter, associated with an independent variable, is the expected amount of change (in form of difference) in the dependent variable for one unit change in the independent variable in question. Instead, the value of the parameter, after anti-log transformation, represents change in the dependent variable in the form of a ratio, given that the independent variable associated with the parameter in question changes by one unit. Therefore, for example, $e^{0.0023} = 1.0023$ will be the ratio of discharge levels after and before precipitation changes by one unit (mm). Or, discharge will increase by 0.23 percent if precipitation increases by one mm. It is worth noting that the estimated parameter only describes the average relation between precipitation and discharge on a monthly basis. For a single rainfall event, the relations are undoubtedly more complex. Similarly, $e^{0.00002} = 1.00002$ will be the ratio of nitrate concentrations after and before nitrogen storage changes by one Mg. In other words, nitrate concentration as NO_3-N will increase by 2 percent if nitrogen storage increases by 1,000 Mg.

When an independent variable and a dependent variable are both log-transformed, the estimated parameter of the independent variable will have the usual interpretation for transformed values, that is, the value of the parameter, associated with the independent variable, is the expected amount of change (in form of difference) in the dependent variable for one unit change (log-transformed) in the independent variable in question. The interpretation of the estimated parameter for the original values of the independent and dependent variables is more complex. Take log-transformed discharge, log(QT), and log-transformed nitrate concentration, log(NO_3N), in the second equation (Table 4) for example. A unit change in log (QT) is equivalent to a new QT value that is **e** times as high as the previous QT, or a change in water discharge by 172 percent. This change in QT will result in a change in logged value of NO_3-N by 0.3295; or $e^{0.3295} = 1.3905$ will be the ratio of nitrate concentration after and before QT changes by 172 percent. In other words, nitrate concentration as NO_3-N will increase by 39 percent if QT increases by 172 percent; or NO_3-N will increase by 2.3 percent if QT increases by 10%.

Seasonal Changes in the Relational Structure

The preceding modeling process was based on the whole data set, or on the whole year basis. The relations revealed by the resultant model in Table 4 may not remain the same all year long. Data analysis over time shows clear seasonal variations in nitrate concentration and its major influencing factors (Table 1). To investigate seasonal variation in the relations, the data set was divided into four subsets based on the following scheme:

Winter: December, January, February;
Spring: March, April, May;
Summer: June, July, August; and
Autumn: September, October, November.

The same model was then separately fit to the data in the four seasonal subsets. The results are given in Tables 5-8.

Winter. In the three winter months (December, January, and February), precipitation had no significant impact on water discharge (p-value = 0.69) (Table 5). Potential evapotranspiration (PET) switched roles from negative to positive in terms of its influence on discharge (cf. Table 4). High PET in the winter would increase instead of decrease discharge as it would on the whole year basis.

Except for lagged values of nitrate concentration, none of the factors in the second equation, air temperature (p-value = 0.41), water discharge (p-value = 0.96), and cumulative change in nitrogen storage (p-value = 0.62), showed significant impact on nitrate concentration in the winter.

In normal years, the dominant form of precipitation in the winter is snow. Because of cold temperature, snow remains on the ground. Usually, water recharge to the aquifer is limited unless abnormal warm temperature causes snowmelt. As such, not surprisingly the model revealed that precipitation did not have significant impact on discharge. On the other hand, PET showed fairly significant and positive influence on discharge (p-value = 0.085). The change of sign in the effect of PET on discharge reflects the role switch of PET from reducing to increasing the amount of water recharged to the aquifer. As PET is derived in part from air temperature, the positive impact of PET on discharge in the winter months reflects the influence of warm temperatures that might cause snowmelt or soil thaw, and in turn recharge events.

As revealed by the model, none of the three factors, discharge, air temperature, and change in nitrogen storage had significant impact on nitrate concentration in the winter. The net input of nitrogen from management point of view is essentially zero in the three winter months. In the meantime, the cold weather keeps mineralization and nitrification processes at a very low level. As such, even when

TABLE 5. Results From Structural Equation Modeling (Winter: December, January, and February).

$$LOG(QT)_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*LOG(QT)_{t-1} + u_{1t}$$

Variable	Parameter Estimate	T-Value	P-Value
P	0.001	0.40	0.6929
PET	0.035	1.79	0.0848
LAG(LOG(QT))	0.870	9.55	0.0001

$$LOG(NO_3N)_t = \alpha_2 + \beta_{21}*LOG(QT)_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*LOG(NO_3N)_{t-1} + u_{2t}$$

Variable	Parameter Estimate	T-Value	P-Value
LOG(QT)	-0.00813	-0.05	0.9592
LAG(T)	0.00468	0.83	0.4132
LAG(N)	0.00001	0.50	0.6223
LAG(LOG(NO3N))	1.21119	5.14	0.0001

Notes: 1. Parameter estimates are those of full information maximum likelihood.
2. R-squares are 0.82 and 0.68 for Equations 1 and 2, respectively.
3. R-square for the equation system is 0.79.

TABLE 6. Results From Structural Equation Modeling (Spring: March, April, and May).

$$LOG(QT)_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*LOG(QT)_{t-1} + u_{1t}$$

Variable	Parameter Estimate	T-Value	P-Value
P	0.005	3.14	0.004
PET	-0.007	-2.86	0.008
LAG(LOG(QT))	0.448	3.28	0.003

$$LOG(NO_3N)_t = \alpha_2 + \beta_{21}*LOG(QT)_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*LOG(NO_3N)_{t-1} + u_{2t}$$

Variable	Parameter Estimate	T-Value	P-Value
LOG(QT)	0.34896	4.10	0.0004
LAG(T)	0.01123	2.40	0.0240
LAG(N)	0.00001	0.88	0.3851
LAG(LOG(NO3N))	0.36104	3.94	0.0006

Notes: 1. Parameter estimates are those of full information maximum likelihood.
2. R-squares are 0.50 and 0.76 for Equations 1 and 2, respectively.
3. R-square for the equation system is 0.60.

abnormal warm winter temperature generates snowmelt and recharge events, little new nitrate is involved in leaching. The effects of winter recharge on nitrate leaching are variable. Rapid snowmelt recharge has a dilution effect on nitrate concentration in water. For winter, the negative sign of the discharge effect on nitrate concentration is an indication of the dilution effect that occurs sometimes, although it is not significant.

Spring. In terms of significance and direction of influence, nearly all the relations in the spring months (March, April, and May) remained the same as those for the whole year, except for change in nitrogen storage (Table 4, Table 6). Change in nitrogen storage a month before did not show significant impact (p-value = 0.39) on nitrate concentration in the current month.

The spring season is transitional in that both snowmelt and rainfall contribute to recharge to the

TABLE 7. Results From Structural Equation Modeling (Summer: June, July, and August).

$$LOG(QT)_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*LOG(QT)_{t-1} + u_{1t}$$

Variable	Parameter Estimate	T-Value	P-Value
P	0.0023	5.69	0.0001
PET	-0.0016	-1.52	0.1399
LAG(LOG(QT))	0.7795	14.72	0.0001

$$LOG(NO_3N)_t = \alpha_2 + \beta_{21}*LOG(QT)_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*LOG(NO_3N)_{t-1} + u_{2t}$$

Variable	Parameter Estimate	T-Value	P-Value
LOG(QT)	0.39916	3.61	0.001
LAG(T)	-0.00062	-0.08	0.934
LAG(N)	0.00001	1.12	0.273
LAG(LOG(NO3N))	0.06385	0.33	0.742

Notes: 1. Parameter estimates are those of full information maximum likelihood.
2. R-squares are 0.90 and 0.71 for Equations 1 and 2, respectively.
3. R-square for the equation system is 0.83.

TABLE 8. Results From Structural Equation Modeling (Autumn: September, October, and November).

$$LOG(QT)_t = \alpha_1 + \gamma_{11}*P_t + \gamma_{12}*PET_t + \gamma_{13}*LOG(QT)_{t-1} + u_{1t}$$

Variable	Parameter Estimate	T-Value	P-Value
P	0.003	3.13	0.0046
PET	-0.004	-2.36	0.0266
LAG(LOG(QT))	1.009	9.48	0.0001

$$LOG(NO_3N)_t = \alpha_2 + \beta_{21}*LOG(QT)_t + \gamma_{24}*T_{t-1} + \gamma_{25}*N_{t-1} + \gamma_{26}*LOG(NO_3N)_{t-1} + u_{2t}$$

Variable	Parameter Estimate	T-Value	P-Value
LOG(QT)	0.37609	4.67	0.0001
LAG(T)	-0.00049	-0.14	0.8924
LAG(N)	0.00004	3.05	0.0056
LAG(LOG(NO3N))	0.36641	2.87	0.0087

Notes: 1. Parameter estimates are those of full information maximum likelihood.
2. R-squares are 0.80 and 0.71 for Equations 1 and 2, respectively.
3. R-square for the equation system is 0.72.

aquifer with the latter gradually replacing the former to become the dominant source. Also, nitrate concentrations steadily increase each month from March to May (Table 1). By contrast, nitrogen storage in the basin continues to decline in February and March as part of the trend starting from December of the previous year. Only in April did the nitrogen storage have a net increase as a result of the beginning of fertilizer application. This indicates that the increase in nitrate concentration in March and April is primarily caused by nitrate leaching from the nitrogen already in storage. Related to increased discharge and temperature, the increase of nitrate concentration in May mainly results from the new nitrogen inputs, that is, the fertilizer application in April.

Summer. In the summer (June, July, and August), rainfall is the only source of water recharge to the aquifer. Precipitation seemingly controlled the variation in discharge and overshadowed the influence of potential evapotranspiration (p-value = 0.14, Table 7). With only precipitation and lagged (antecedent) discharge appearing significant in the first equation, the proportion of variation in discharge in the summer explained by the model is 90 percent, which is higher than that on the whole year basis (71 percent).

Discharge, in turn, was the dominant factor in regard to variation of nitrate concentration. With discharge being the only significant factor in the second equation, the proportion of variation in nitrate concentration in the summer explained by the model is still higher than that for the whole year (71 percent vs. 65 percent).

Because of increased frequency and intensity of recharge events and nitrification processes, nitrate leaching to the ground water may appear at the outlet of the basin at a faster pace in the summer than the rest of the year. As such, air temperature in the current month may be more responsible for the observed nitrate concentration than air temperature a month before. To test for this assumption, the same model, except for the substitution of current month's air temperature for the lagged observation, was then fitted again to the data for the summer months. The result showed significant and positive impact of air temperature on nitrate concentration (t-value = 2.12 and p-value = 0.04). This is quite a turn-around compared to the lagged observation of air temperature (t-value = -0.08 and p-value = 0.93).

Increased intensity of nitrification in the summer results in greater amounts of available nitrate for potential leaching. When significant precipitation and resultant recharge events occur, a large amount of nitrate is lost to the ground water and surface water. As shown in Table 1, June and July have the highest values of nitrate concentration. In June, rising nitrate concentrations can be caused by incremental increase in nitrogen storage as a result of fertilizer application in May. On the other hand, monthly balance of nitrogen between input and output was consistently negative from June to August, indicating loss of nitrogen from the basin storage because this is also the period of greatest plant uptake. This suggests that high nitrate concentration in July was primarily a function of nitrogen already in storage.

Although placed in the same season with June and July, August is quite different from the other two months in the summer. A prominent drop in nitrate concentration is typically observed for August (Table 1). This may partly be caused by large amount of nitrogen loss (nitrogen uptake by plants and losses in water) in the previous month (July), the largest in the whole year (Table 1). In other words, the decline in nitrate concentration in August was related to the decrease in nitrogen storage in July. In addition, reduced discharge in August, related to low precipitation and high PET, was also a major factor (Table 1).

Autumn. In the three autumn months (September, October, and November), in terms of significance and direction of influence, nearly all the relations remained the same as those on the whole year basis (Table 8), except the air temperature that did not show significant impact on nitrate concentration (p-value = 0.89). As with the spring, the autumn season is also transitional, but in the opposite direction. Temperature and precipitation tend to decline steadily in a monotonic fashion. Rainfall is still the dominant, but not the only form of precipitation. In some years, November may see snowfall. Snowmelt, however, is not an important source of water recharge to the aquifer. The influence of temperature on evapotranspiration still overshadows its impact on snowmelt, as indicated by the negative sign of t-value for PET in Table 8.

Despite a steady decline in temperature in the autumn, nitrate concentration did not drop in this season compared to that in August (Table 1). Thus, temperature seemed to have no significant influence on nitrate concentration during this period of time. One of the reasons for the stable nitrate concentration is probably the consistent net increase in nitrogen storage in those months as a result of the decline in plant uptake and some fertilizer application in this season. There may also be a reduction in intensity of denitrification with declining temperature and biotic activities.

The classification of the four seasons adopted in this study does not imply that the same relations hold for each month within the same season. Instead, the causal relations may change, more or less, between some months. Thus, a better way to investigate seasonal change in the structural equation model may be to test the model on a monthly basis. The constraint of available data, however, limits the viability of such an approach at this time.

CONCLUSIONS

This study shows that for given hydrogeological settings, nitrogen management practices in agricultural production and climate are the two most important factors that affect the dynamics of nitrate contamination in ground water in an agricultural drainage basin. The long-term trend of nitrate concentration is closely related to the nitrogen input to the basin primarily determined by nitrogen management practices. The potential effects of nitrogen management, however, are contingent on the variations of climate.

One of the major goals in the Big Spring Basin project is to be able to document improvements in water quality (i.e., reduced NO_3-N concentrations/loads) in relation to improved nitrogen management. This study provides some important insights. The study suggests the continued growth in nitrogen storage in the basin, despite the decreased fertilizer nitrogen loading as a result of implementation of improved nitrogen management practices. This means that further reduction in nitrogen input from agricultural production is likely needed to substantially improve the water quality. The study also shows that the improvements in water quality related to improved nitrogen management are often overshadowed by the impact of climate, especially in extremely dry or wet years. The best example is year 1991 when the record-high nitrate concentration was observed despite the relatively low nitrogen input in that year and a number of previous years.

Structural equation modeling applied in this study provides a quantitative perspective on the effects the influencing factors have on NO_3-N concentration. As suggested by the model, on average, a 1,000 Mg increase/decrease in nitrogen storage (close to annual net input of nitrogen) will result in a 2 percent increase/decrease in NO_3-N concentration; while a change in water discharge by only 10 percent will cause a change in NO_3-N concentration by 2.3 percent. Discharge variations of 10 to 100 percent from year to year are common (Table 2). This implies that the variations of climate (especially precipitation) and hydrology (measured as water discharge) have much greater impacts on the nitrate dynamics than the changes in nitrogen input. This explains why the effects of improved nitrogen management are often overshadowed by the impact of climatic variations.

This study also reveals significant seasonal variation in the relations between nitrate concentration and its influencing factors. That is, the relations specified and confirmed by the structural equation model did not remain the same all year long. Instead, those relations varied from season to season in terms of significance and nature (positive or negative) of influences. The pattern of seasonal variation in the relations is closely related to the seasonal variation of climate. As such, future assessment of management practices and resultant water quality should consider the impact of short- and long-term climate dynamics.

Since the Big Spring Basin is a good working example of agroecosystems on a watershed scale, the findings and conclusions from this study are applicable to other agricultural drainage basins. They can also be used in the future studies of nitrate contamination in ground water as related to agricultural production in different geographic areas and regions. The methods and techniques of analysis and modeling applied in this research can also be used in other environmental investigations.

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