

A STOCHASTIC MODEL CHARACTERIZING
THE DYNAMICS OF NITROGEN
CONCENTRATION IN AN ECOSYSTEM

by

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INTRODUCTION

Particle movement in ecosystems is of interest to scientists, engineers and investigators in many different disciplines. Examples might include petroleum spills, chemical reactions that occur over time, or the dispersion of matter in the atmosphere.

Compartmental analysis has been used in ecosystem particle dispersion modelling for a number of years (Bloom et al., 1971; Dahlman et al., 1969; Eberhardt and Hanson, 1969; Hannon, 1973; Martin et al., 1969; Gore and Olson, 1967; Kelly et al., 1969; Cale, 1975; Finn, 1977). For the most part these models have been deterministic where the random or stochastic aspects of the process or ecosystem have been largely ignored. The process of particulate matter subjected to dispersion in a fluid environment is a random process. As such, its behavior is subject to natural laws requiring probabilistic modelling and interpretation. Stochastic models often provide an adequate description of such processes over time.

In recent years interest has developed in stochastic models for flow systems. Markov Chains have been the principle modelling tool employed (Barber, 1978 a, b; Horn, 1975; Kamota et al., 1976).

This report investigates the application of a stochastic model in describing the distribution of nitrogen particles in a perennial stream of Kings Creek on the Konza Prairie in North Central Kansas.

One aspect of the model was suggested by Nassar et al., (1984) as a methodology for modelling the concentration of particulate matter in a filter system. In this report we extend the model and apply it to an ecosystem that is traditionally viewed other than as a filter or a conduit for moving particulate matter. The model seems adequate in

describing the observed nitrogen concentration over space and time, assuming only those characteristics that were consistent with the natural ecological system under observation.

The ecosystem system or stream is arbitrarily divided into 'n' compartments. Nitrogen enters the stream into the first compartment. Each chamber will be assumed to have its own uptake parameter, μ_i (loss of nitrogen molecules due to algae uptake or leaching) and there would be an intensity, $k_{i,i+1}$, associated with the transition of molecules from compartment i to compartment $i+1$, ($i = 1, 2, \dots, n$). The interest is in predicting the molecular concentration over space and time in the stream.

MODEL

Let

$$\mu_i(t)\Delta t + o(\Delta t) = \text{Pr(A particle or molecule in compartment } i \text{ at time } t \text{ will vanish through uptake at time } t+\Delta t).$$
(1)

$$k_{i,i+1}(t)\Delta t + o(\Delta t) = \text{Pr(A molecule in compartment } i \text{ at time } t \text{ will move to state or compartment } i+1 \text{ downstream at time } t+\Delta t).$$
(2)

$$1 - k_{i,i+1}(t)\Delta t - \mu_i(t)\Delta t + o(\Delta t) = \text{Pr(A molecule in state } i \text{ at time } t \text{ will remain in the same state at time } t+\Delta t).$$
(3)

Further, define the transition probability,

$$P_{ij}(\tau, t) = \text{Pr (A molecule in state } i \text{ at time } \tau \text{ will be in state } j \text{ at time } t, \\ i, j = 1, 2, \dots, n) \quad (4)$$

The solution for $P_{ij}(\tau, t)$ when the intensities μ_i and transitions $k_{i, i+1}$ are constant over time may be expressed (Nassar, 1986) as

$$P_{ij}(\tau, t) = \frac{j}{k_{i, i+1} \cdot k_{i+1, i+2} \cdots k_{j-1, j}} \cdot e^{[\rho_j(t-\tau)]} \prod_{\substack{m=i \\ \ell \neq m}}^j (\rho_\ell - \rho_m) \quad (5)$$

Where

$$\rho_\ell = -(k_{\ell, \ell+1} + \mu_\ell) ; \ell = 1, 2, \dots, n \quad (6)$$

and

$$P_{ii}(\tau, t) = \exp[\rho_i(t - \tau)]. \quad (7)$$

When $\mu_i(t)$ and $k_{i, i+1}(t)$ are continuous functions of time the solution to the $n \times n$ matrix

$$\underline{P}[\tau, t] = (p_{ij}(\tau, t))$$

may be expressed as

$$\underline{P}(\tau, t) = \underline{I} + \int_{\tau}^t \underline{P}[\tau, \xi] \underline{K}(\xi) d\xi \quad (8)$$

where \underline{I} is the identity matrix and \underline{K} a bidiagonal $n \times n$ matrix of the form

$$\underline{K} = \begin{pmatrix} k_{11} & k_{12} & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & k_{22} & k_{23} & 0 & \dots & 0 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 0 & k_{n-1, n-1} & k_{n-1, n} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & k_{n, n} \end{pmatrix}.$$

Equation (8) may be solved iteratively according to the matrix sequence,

$$\begin{aligned} \underline{G}_0 &= \underline{I} \\ \underline{G}_{-m+1} &= \underline{I} + \int_{\tau}^t \underline{G}_{-m} \underline{K}(\xi) d(\xi). \end{aligned} \quad (9)$$

If $\underline{K}(\xi)$ is constant over time, (8) reduces to the time homogeneous solution of equation (5).

Let the concentration of nitrogen in the stream at the point of entry into compartment 1 (i.e., $i = 1$) be denoted by

$$C_0(s); \quad s \geq \tau \geq 0.$$

It is seen that the expected nitrogen concentration in compartment j ($j = 1, 2, \dots, n$) at t is

$$E[C_j(t)] = \int_{\tau \rightarrow \infty}^t C_0(s) p_{1j}(s, t) k_{j, j+1} ds, \quad j=1, 2, \dots, n-1. \quad (10)$$

Here t approaches infinity since we assume that the nitrogen concentration in the perennial stream has reached a limiting distribution.

DATA SOURCE

The data employed in this study were collected by Tate (1985). Measurements of nitrogen concentration ($\mu\text{g}/\text{liter}$) were collected at selected sites along a perennial reach of the King's Creek in the Konza Prairie Preserve (Fig. 1). Collection commenced in October 1983 and continued weekly through October 1984.

A "reach" is a continuous expanse of moving surface water, that is, a creek. A perennial reach is a creek that flows throughout the year. Water enters a reach in the form of runoff from rain fall, snow fall, and seepage from underground water sources. A "seep" is a point where underground water courses intersect the creek and become a part of the input water source. If the number of seeps is sufficient, and if their flow is continuous, the waterway will maintain a year-round current flow.

Nitrogen is introduced into the creek carried by input water sources, that is as solutes in both runoff water and underground seepage. Ground water washes nitrogen formed by decaying organic material on the surface of the drainage area. Underground water collects nitrogen while percolating through the soil. After seeping through porous soil, percolation water may encounter a non-porous stratum such as clay or bedrock, in which case flow commences laterally through the last porous stratum. When a water bearing gravel or sand

channel encounters a creek, the water and its captive nitrogen enters the stream as part of the input cycle.

Runoff water is more transient in nature and could contribute significantly to observed perturbations in the nitrogen content. This source of moisture is available any time the drainage area receives rain. Entry to the reach is effected by way of tributaries and down banks. Rainfall water sources quickly exhaust themselves. Water flowing through the soil takes much longer to reach the stream than the surface runoff. Depending on the topography of the drainage area, underground water may require weeks, months or many years to exit. Concentrations of nitrogen from such sources are functions of previously existing organic matter and the length of time from rain to exit. This introduces a variable time lag from rainfall to stream contribution and is responsible for cyclical patterns in the measurements.

King's Creek ranges over a three kilometer long area before it finally sinks into the ground. The point at which the stream disappears is defined as the discharge location or sink. Progressing upstream from the sink, the farthest seep location that exhibited year round flow was located, and thus defined as the "source". All other input water sources between the "source" and the final sink were referenced by distance downstream from the "source". Using this technique, the sink is located 578.7 meters from the source.

There were several small tributaries (none perennial) and several identifiable seeps downstream from the source. Observations were collected at each of these ancilliary sources, and at a short distance downstream.

MODEL FITTING

To simplify the model equations, modelling was begun at the first point downstream from the last source of water input. This insured that the continuous nitrogen input entered the stream flow through the first compartment only. Thus, the original compartment boundary was for measurements taken at distance 292. Measurements were also recorded at 345, 429, 474 and 578 meters from the source. These points were defined as the end points of our arbitrary compartments.

Since the stream is perennial with continuous flow it is clear that time, in terms of the model, must be taken as infinite. With constant input rate and intensities, one expects that nitrogen concentration attains a limit at each point or compartment down the stream. If either the input rate or the intensities are functions of time, namely cyclic in nature, it follows that the limiting nitrogen concentrations would not be constant but rather cyclic. Plots of the nitrogen concentrations at the compartment boundaries suggest that the data is cyclic with a primary phase of twelve months and that the stream is at a steady state.

Spectral analysis for each compartment boundary suggested that the cyclical patterns were very likely the only discernable components in the data. A backward elimination procedure was used to select those components that best fit the data. The models were thus obtained using the General Linear Models Procedure (SAS, 1982) and residual plots generated. Removal of the significant cyclical components yielded random appearing error plots.

In fitting the stochastic model to the data it is logical to assume that the nitrogen input rate is a cyclical function of time, since it depends to a large extent on seasonal environmental conditions. It is possible that nitrogen uptake in the stream (intensity parameter μ_i) is a function of time due to the growth of algae which is seasonal. The data collected, however, did not have any measurement on algae growth or concentration in the stream, nor on the flow rate of the stream from which one might discern the transition intensities (K_{ij}) over time. It seemed to us that the data did not warrant fitting complicated models where the input rate and intensities are taken to be a cyclical function of time. As a start we considered the case where only the input rate of nitrogen is a cyclical function of time with the μ_i 's and k_{ij} 's held constant.

For a general cyclical function we considered the model,

$$\begin{aligned}
 C_o(t) &= \alpha + \sum_i \beta_i \cos(\omega t + \theta_i) + e \\
 &= \alpha + \sum_i \beta_i \cos(\theta_i) \cos(\omega t) - \sum_i \beta_i \sin(\theta_i) \sin(\omega t) + e \quad (11)
 \end{aligned}$$

where

- α = The intercept
- β_i = The i th amplitude,
- t = The time in days,
- ω_i = The phase angle = $2\pi i/375$, $i=1,2,\dots,n$,
- θ_i = The shifts in the phase angle, assumed to be independent and uniformly distributed over $(0, 2\pi)$.

$e \sim N(0, \sigma^2)$

Equation (11) was fitted to the observed concentration $\hat{C}_0(t)$ using multiple regression and estimates of the β_i 's and θ_i 's were obtained.

From equations (10) and (11), assuming $k_{j,j+1}$ to be independent of time, one may obtain the predicted concentration, $E[C_j(t)]$, by integration, for each of the locations downstream from the source. The integral in (10) with $C_0(s)$ as given in (11) may be expressed in general as

$$E[C_j(t)] = A_j + \sum_i D_{ij} \cdot \sin(\omega_i t) + \sum_i E_{ij} \cdot \cos(\omega_i t), \quad (12)$$

where A_j , D_{ij} and E_{ij} are constants which can be expressed as functions of the intensities (μ_i , $k_{i,i+1}$) of the model and the constants α , β_i and θ_i of expression (11). For instance, we can write

$$E[C_1(t)] = \frac{\alpha k_{12}}{k_{12} + \mu_1} + \sum_i \left[\frac{\omega_i k_{12} \beta_i \cos(\theta_i) - k_{12} \beta_i \sin(\theta_i) (k_{12} + \mu_1)}{[k_{12} + \mu_1]^2 + \omega_i^2} \right] \sin(\omega_i t) \\ + \sum_i \left[\frac{(k_{12} + \mu_1) k_{12} \beta_i \cos(\theta_i) + k_{12} \beta_i \sin(\theta_i)}{[k_{12} + \mu_1]^2 + \omega_i^2} \right] \cos(\omega_i t). \quad (13)$$

It is interesting to note that $E[C_j(t)]$ has the same functional form as $C_0(t)$ and is also cyclical. From the coefficients in (12) one may estimate the intensities. Further, one may derive the autocovariance function $[\sigma_j(h)]$ of nitrogen concentration at any compartment j , in the

limit. This may be expressed as

$$\sigma_j(h) = \{E_\theta \int_{t \rightarrow \infty} [\sum_i \beta_i \text{Cos}(\omega_i t + \theta_i) p_{ij}(t-s) k_{j,j+1}] \cdot [\sum_i \beta_i \text{Cos}(\omega_i t + \omega_i h + \theta_i) p_{ij}(t+h-s) k_{j,j+1}] ds\} \quad (14)$$

where

E_θ - Expectation with regard to θ which has a uniform distribution on the interval $(0, 2\pi)$.

This leads to the general form of the expression for the autocorrelation function, $\rho_j(h)$.

$$\rho_j(h) = \left(\frac{r}{\sum_{\ell=1}^r} \frac{\exp(-A_\ell h)}{A_\ell} \right) \left(\frac{\sum_i \beta_i^2 k_{i,j+1} \text{Cos}(\omega_i h)}{\sum_i \beta_i^2 k_{j,j+1}^2 + \sigma_e^2} \right) \quad (15)$$

where

$$r = j(j+1)/2.$$

A_ℓ , k_ℓ , and β_i are constants and σ_e^2 is the error variance in (11).

For example, if $j = 1$

$$\rho_1(h) = \frac{\exp(-Ah)}{2A} \frac{4 \sum_{i=1}^4 \beta_i^2 k_{i2} \text{Cos}(h\omega_i)}{\sum_i \beta_i^2 k_{i2}^2 + \sigma_e^2} \quad (16)$$

It is seen from (15) that $\rho_j(h)$ is a linear combination of sinusoidal

oscillations dampened over time by the exponential terms.

RESULTS AND CONCLUSIONS

The model in (12) was fitted to the observed nitrogen concentrations $\hat{C}_j(t)$. The model selected for distance 292 (entry into compartment one) was fitted for each subsequent downstream location. Parameter estimates for each of the five locations appear in tables (1-5) in the appendix of this report. After the generalized model was fit, residual errors were estimated at each location. The plots of the prediction equations appear to fit the data, and the residuals generally lack any significant trend or pattern (Fig. 2 - 6).

Coefficients for some of the four sine and cosine terms in the model were not significant for certain locations. This may be due to local perturbations in the observed $\hat{C}_j(t)$ concentrations due to runoff water, or it may suggest that the μ_i and k_{ij} parameters are functions of time, changing according to existing physical and environmental conditions. An experimental situation designed to measure time changes in nitrogen uptake and changes in stream flow rates could lead to a better fit of the model to the data.

No attempt was made to fit the autocorrelation function in (16) to the data. The S.A.S. autoregressive integrated moving average (ARIMA) procedure was employed to estimate correlations for up to 46 lags (Figs. 7 - 11). It is clear from these figures that the observed autocorrelation exhibited sinusoidal oscillations dampened over time as predicted by the model.

The model is both general and flexible. It has the capability of estimating many more parameters than are used in this report. For instance, flow intensities ($k_{i,i+1}$) and uptake parameters (μ_i) can be modelled as either constants or as functions of time.

It would be of interest to extend the model to the whole stream where nitrogen enters at several compartments downstream from the source also to consider the concentration of nitrogen entering the streams as a random variable. Measurements of nitrogen concentrations, uptake by algae and volumetric flow rates at different sections of the stream, over a time period longer than one year would be desirable for a better understanding of the dynamics of the process and a better fit of the model to the data.

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APPENDIX

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TABLE 1. Estimated coefficients of equation (12), filled nitrogen concentrations at a distance of 292 meters.

$$\begin{aligned}
 N_{33} = & B_0 + C_1 * \cos(2 * \pi * T / 375) + S_1 * \sin(2 * \pi * T / 375) \\
 & + C_2 * \cos(4 * \pi * T / 375) + S_2 * \sin(4 * \pi * T / 375) \\
 & + C_3 * \cos(6 * \pi * T / 375) + S_3 * \sin(6 * \pi * T / 375) \\
 & + C_4 * \cos(8 * \pi * T / 375) + S_4 * \sin(8 * \pi * T / 375).
 \end{aligned}$$

R-SQUARE: 0.7377

MEAN SQUARE ERROR: 40.56

OBS: 50

PARAMETER	ESTIMATE	STANDARD ERROR
B0	15.9504	0.9110
C1	12.7296	1.2749
C1	- 1.2445	1.3010
C2	- 0.4453	1.2858
S2	- 5.2167	1.2743
C3	- 4.2226	1.2692
S3	- 4.4951	1.3132
C4	- 2.7730	1.2233
S4	- 1.2390	1.3573

TABLE 2. Estimated coefficients of equation (12), filled nitrogen concentrations at a distance of 345 meters

$$\begin{aligned}
 N_{33} = & B_0 + C_1 * \cos(2 * \pi * T / 375) + S_1 * \sin(2 * \pi * T / 375) \\
 & + C_2 * \cos(4 * \pi * T / 375) + S_2 * \sin(4 * \pi * T / 375) \\
 & + C_3 * \cos(6 * \pi * T / 375) + S_3 * \sin(6 * \pi * T / 375) \\
 & + C_4 * \cos(8 * \pi * T / 375) + S_4 * \sin(8 * \pi * T / 375).
 \end{aligned}$$

R-SQUARE: 0.7238

MEAN SQUARE ERROR: 40.69

OBS: 50

PARAMETER	ESTIMATE	STANDARD ERROR
B0	13.8772	0.9060
C1	11.0724	1.2565
S1	- 0.1874	1.3002
C2	- 0.9270	1.2754
S2	- 4.0171	1.2796
C3	- 4.3919	1.2699
S3	- 2.0457	1.2350
C4	- 3.7376	1.2350
S4	- 0.0021	1.3221

TABLE 3. Estimated coefficients of equation (12), fitted to nitrogen concentrations at a distance of 429 meters.

$$\begin{aligned}
 \text{NO}_3 = & B_0 + C_1 * \cos(2 * \pi * T / 375) + S_1 * \sin(2 * \pi * T / 375) \\
 & + C_2 * \cos(4 * \pi * T / 375) + S_2 * \sin(4 * \pi * T / 375) \\
 & + C_3 * \cos(6 * \pi * T / 375) + S_3 * \sin(6 * \pi * T / 375) \\
 & + C_4 * \cos(8 * \pi * T / 375) + S_4 * \sin(8 * \pi * T / 375).
 \end{aligned}$$

R-SQUARE: 0.3541

MEAN SQUARE ERROR: 42.96

OBS: 50

PARAMETER	ESTIMATE	STANDARD ERROR
B0	8.0853	0.9303
C1	3.6280	1.2710
S1	3.6579	1.3365
C2	- 2.0135	1.3110
S2	- 1.7707	1.3162
C3	- 1.8887	1.3053
S3	- 1.0454	1.3207
C4	- 1.2601	1.2575
S4	0.6257	1.3540

TABLE 4. Estimated coefficients of equation (12), fitted to nitrogen concentrations at a distance of 429 meters.

$$\begin{aligned}
 \text{NO}_3 = & B_0 + C_1 * \cos(2 * \pi * T / 375) + S_1 * \sin(2 * \pi * T / 375) \\
 & + C_2 * \cos(4 * \pi * T / 375) + S_2 * \sin(4 * \pi * T / 375) \\
 & + C_3 * \cos(6 * \pi * T / 375) + S_3 * \sin(6 * \pi * T / 375) \\
 & + C_4 * \cos(8 * \pi * T / 375) + S_4 * \sin(8 * \pi * T / 375).
 \end{aligned}$$

R-SQUARE: 0.3952

MEAN SQUARE ERROR: 31.34

OBS: 50

PARAMETER	ESTIMATE	STANDARD ERROR
B0	6.5011	0.7902
C1	2.4698	1.0887
S1	4.0101	1.1411
C2	- 2.1084	1.1035
S2	1.9840	1.1231
C3	- 1.3046	1.0780
S3	1.0240	1.1273
C4	- 0.9040	1.0575
S4	- 0.0830	1.1601

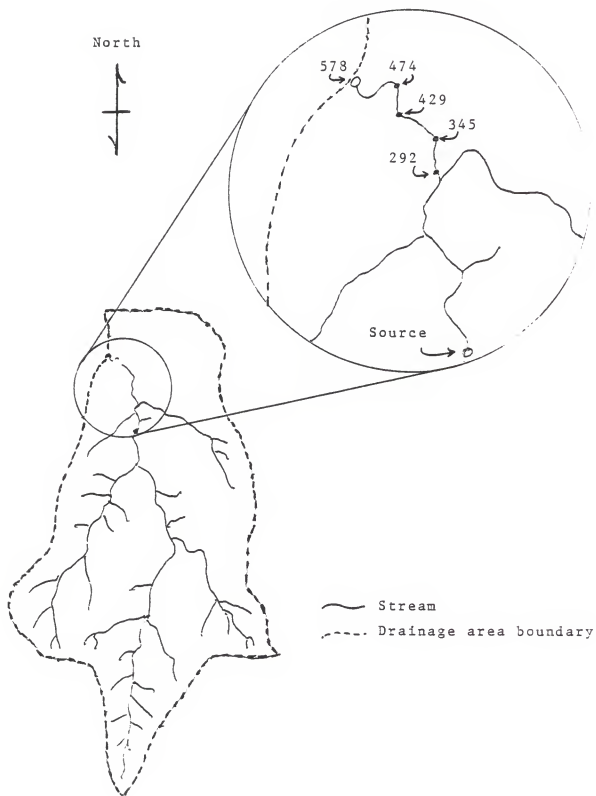
TABLE 5. Estimated coefficients of equation (12, filled to nitrogen concentrations at a distance of 578 meters. 18

$$\begin{aligned}
 \text{NO}_3 = & \text{B0} + \text{C1} * \text{COS}(2 * \text{PI} * \text{T} / 375) + \text{S1} * \text{SIN}(2 * \text{PI} * \text{T} / 375) \\
 & + \text{C2} * \text{COS}(4 * \text{PI} * \text{T} / 375) + \text{S2} * \text{SIN}(4 * \text{PI} * \text{T} / 375) \\
 & + \text{C3} * \text{COS}(6 * \text{PI} * \text{T} / 375) + \text{S3} * \text{SIN}(6 * \text{PI} * \text{T} / 375) \\
 & + \text{C4} * \text{COS}(8 * \text{PI} * \text{T} / 375) + \text{S4} * \text{SIN}(8 * \text{PI} * \text{T} / 375).
 \end{aligned}$$

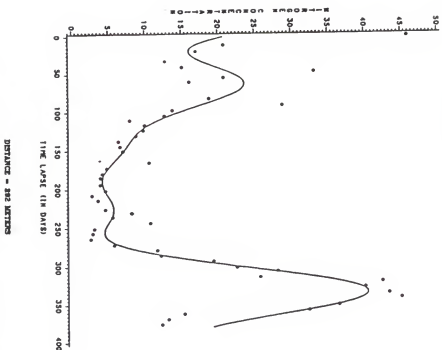
R-SQUARE: 0.4204 MEAN SQUARE ERROR: 34.51 OBS: 41

<u>PARAMETER</u>	<u>ESTIMATE</u>	<u>STANDARD ERROR</u>
B0	10.1292	1.6651
C1	7.3475	2.3891
S1	4.4731	2.2403
C2	3.2120	2.0420
S2	1.9073	2.4933
C3	2.1469	2.1545
S3	1.1248	2.3102
C4	1.1232	2.0576
S4	0.8003	2.2952

Figure 1. King's Creek and Konza Prairie drainage area.



LOT OF PREDICTED AND
OBSERVED CONCENTRATIONS



LOT OF ESTIMATED RESIDUALS

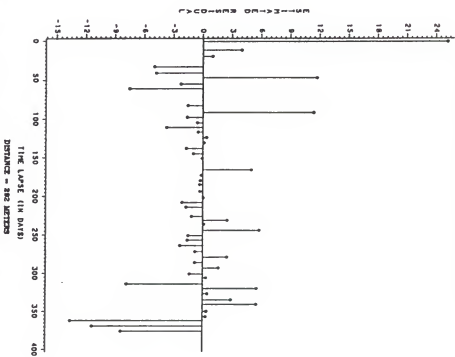
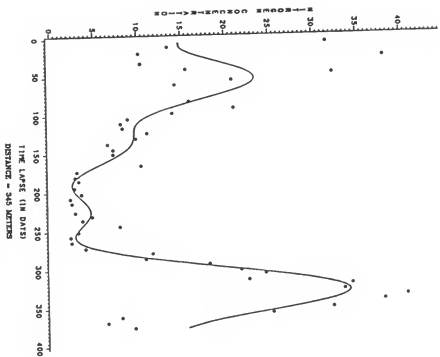


FIGURE 2. Plot of predicted nitrogen concentrations from the model in Table 1 and plot of the residuals.

PLOT OF PREDICTED AND
OBSERVED CONCENTRATIONS



PLOT OF ESTIMATED RESIDUALS

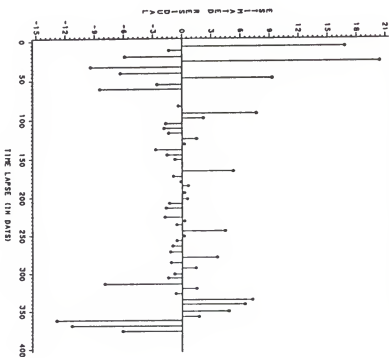
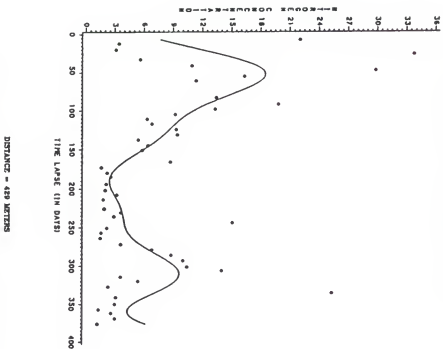


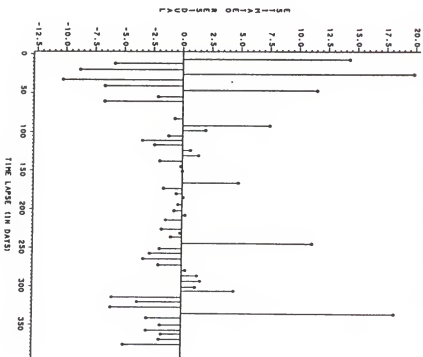
FIGURE 3. Plot of predicted nitrogen concentrations from the model in Table 2 and plot of the residuals.

PLOT OF PREDICTED AND
OBSERVED CONCENTRATIONS



DISTANCE - 429 METERS

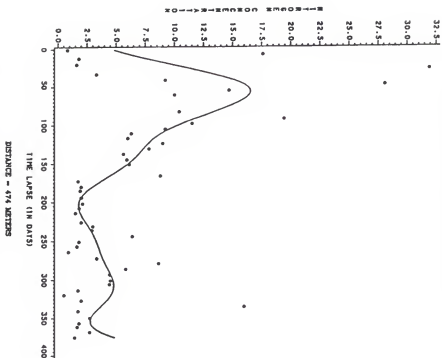
PLOT OF ESTIMATED RESIDUALS



DISTANCE - 429 METERS

FIGURE 4. Plot of predicted nitrogen concentrations from the model in Table 3 and plot of the residuals.

LOT OF PREDICTED AND
OBSERVED CONCENTRATIONS



LOT OF ESTIMATED RESIDUALS

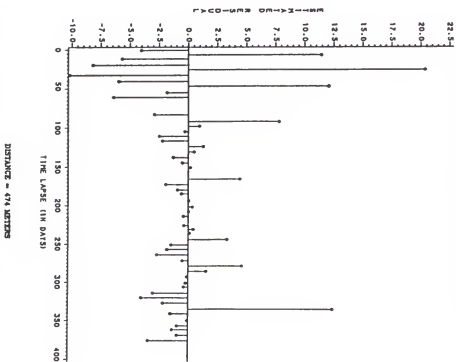
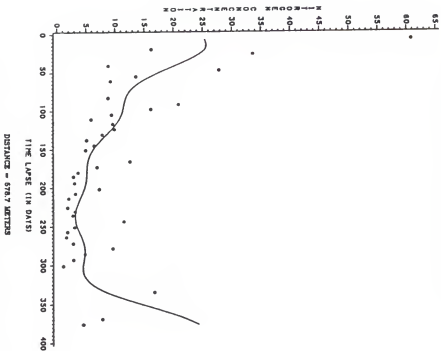


FIGURE 5. Plot of predicted nitrogen concentrations from the model in Table 4 and plot of the residuals.

PLOT OF PREDICTED AND OBSERVED CONCENTRATIONS



PLOT OF ESTIMATED RESIDUALS

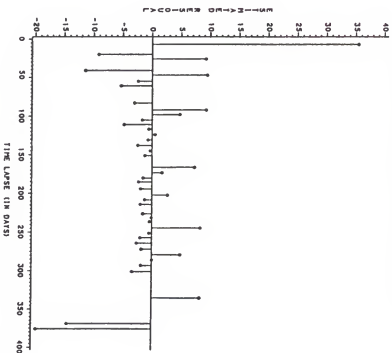
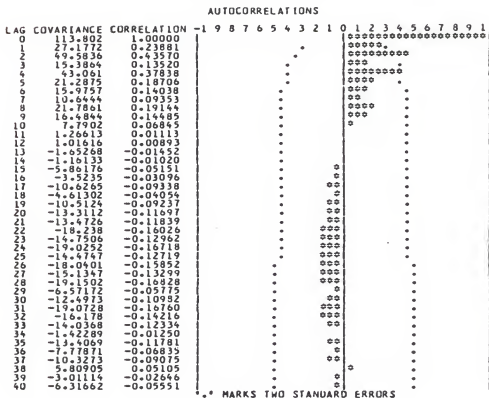


FIGURE 6. Plot of predicted nitrogen concentrations from the model in Table 5 and plot of the residuals.

FIGURE 11. Observed autocorrelations for distance 578.



ACKNOWLEDGMENTS

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A STOCHASTIC MODEL CHARACTERIZING
THE DYNAMICS OF NITROGEN
CONCENTRATION IN AN ECOSYSTEM

by

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AN ABSTRACT OF A MASTER'S REPORT

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requirements for the degree

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1987

ABSTRACT

This report investigates the application of a stochastic model to characterize and predict the dynamics of nitrogen concentration in an ecosystem. The model is derived and adapted to describe a steady state, cyclical system. Tests of adequacy are performed by fitting the model to the data and generating residual plots. A general form of the autocorrelation function is derived and found to be consistent with the observed autocorrelations in the data.