A Systems Approach to an Analysis of the Terrestrial Nitrogen Cycle

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ABSTRACT

In an interdisciplinary study, a new methodology for analysis of environmental systems is being applied to the terrestrial nitrogen cycle. It has already resulted in an informative, qualitative description of this complicated system and its components. With this system definition, we plan to develop a mathematical simulation of the dynamics of the nitrogen cycle in both forested and agricultural ecosystems. Initial results from on-going experimental and modeling studies in soil chemistry and soil physics have been encouraging. A critical evaluation of the final simulation model, using field data obtained from an extensive system monitoring program, will be a rigorous test of the feasibility and merit of the proposed systems method.

Introduction

Development and evaluation of measures for environmental protection require a quantitative knowledge both of the individual processes which

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make up a particular ecological system, and of the interrelationships between these processes. This knowledge is essential to elucidate the cause and effect pathways and to identify the most suitable means of attacking the problem. The detailed investigation of fundamental biological processes is the responsibility of the biological scientist, but the analysis of an entire ecological system requires the cooperation of physical scientists, statisticians, and engineers as well. Integration of their diverse contributions is achieved through systems analysis—a systematic mathematical approach to large, complex problems.

This paper is a progress report on an interdisciplinary study of this type. A diverse team of scientists and engineers is building a mathematical model for simulating the movement and biochemical transformation of inorganic and organic nitrogen species in selected soil systems. With such a model, we can analyze and evaluate the role played by soil drainage in the nitrate pollution of groundwater supplies and the eutrophication of our natural water systems, as well as predict, quantitatively, the effects of nitrogenous fertilizers and of changing land-use patterns. The model development combines the theory and analysis of the statistician and the chemical engineer with the experimental methods and results of the soil physicist and soil chemist. This systems approach is general enough to be useful in analyzing many environmental systems.

First we describe the methods used in our systems analysis, and define the terrestrial nitrogen cycle which is the basis of the ecosystems to be studied. Some details follow on the two particular systems to be investigated—deciduous forest and sandy soil. Next we describe the framework and basis of the mathematical model to be used. Our discussion closes with some details of the modeling and experimental studies of the soil physics and soil chemistry involved.

Systems Analysis

The numerous texts and articles on systems analysis contain many definitions of the subject. Most of these are conceptual and do not provide the layman or uninformed scientist with a fundamental understanding of the systems approach to problem solving. The following functional or operating definition of systems analysis is probably more useful. According to Nadler,² a system is a collection of real life phenomenon that possesses the seven elements defined in Table 1. In this context, systems analysis is the logical and comprehensive specification and study of these seven elements, both individually and collectively.

The systems approach can be clarified still further by consideration of a specific method for implementing a logical and comprehensive study of a

Table 1. The Seven Elements of a System*

1. Function	Objective which the system attempts to achieve.
2. Inputs	Materials and energy which are processed by the system to arrive at the outputs.
3. Outputs	Desired and undesired material and energy products of the system.
4. Sequence	Interrelationships among the component processes of the system, and the order in which they operate, such that the inputs are converted to the outputs.
5. Environment	Physical surroundings within which the system operates.
6. Physical agents	Material (non-human) resources which operate in at least one step of the system sequence, but which do not become a part of the output.
7. Human agents	Human resources which operate in the system sequence.

^{*}Adapted from Nadler.2

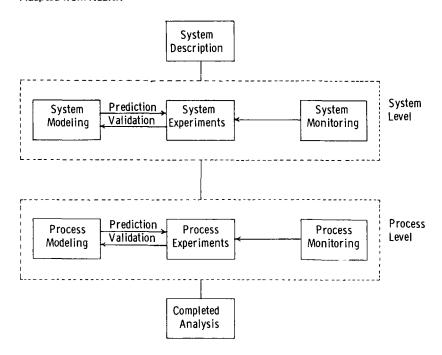


Figure 1. A schematic representation of a method for systems analysis.

system. Figure 1 is a schematic representation of such a method suggested in part by Loucks et al.³ The first required step is a complete description of the seven system elements described in Table 1. This is followed by investigations at the system and process levels. While the end result of a systems analysis is usually an integrated system model, it must be emphasized that it can be no better than its component process models.

The iterative, feedback nature of systems analysis (Figure 1) is portrayed in more detail in Figure 2, which has been adapted from Van Dyne.⁴ An investigator's definition and model of a system and its component processes must always be subject to alteration. As more is learned about the system during the analysis, the specification and models of the system can be improved by appropriate modification based on experimentally obtained evidence.

Another concept to be clarified is that of models and modeling. Nadler² defines a model as an abstraction of a real life phenomenon which is used as a means of representing some part of a defined system. This model need not be mathematical in form. In fact, during the definition phase of a systems analysis, it is usually in a schematic form.

A mathematical model is the usual formal objective of a modeling study. It consists of one or more mathematical relationships, which predict the values of a set of dependent variables Y, as a function of a set of independent variables X and parameters k. Thus, the general form of a mathematical model is the following:

$$Y = f(X,k) \tag{1}$$

At the initiation of a modeling study the set of the dependent variables of interest has already been specified. A prior specification of f, X, or k, however, is not required. Indeed, determination of any combination of these three factors is the goal of the study itself. Hunter⁵ has defined the four general classes of modeling studies presented in Table 2. The actual techniques required in these studies vary from well-developed theories such as linear regression,⁶ to comparatively new methods, such as model discrimination,⁷ for which the theory is still being developed.

System Definition of the Terrestrial Nitrogen Cycle

The first element of the system to be specified, as indicated in Table 1, is the function of the terrestrial nitrogen cycle. This can be defined as maintenance of the balance between atmospheric and lithospheric nitrogen by the circulation, transformation, and accumulation of the various forms of inorganic and organic nitrogen through the biotic and abiotic segments of the terrestrial environment.

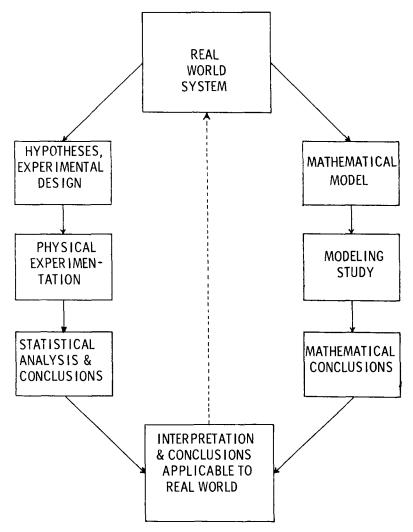


Figure 2. The interdependence of experimentation and modeling in systems analysis adapted from an illustration in Van Dyne.⁴

A discussion of the inputs and outputs to this system can be facilitated by introducing the carrier concept. A carrier is a material that can transport or store one or more nitrogen compounds. The concentration of a given nitrogen compound in a carrier is defined such that, when we multiply the concentration by an appropriate measure of the bulk amount of the carrier, we obtain the total amount of the given nitrogen compound in the carrier. The different forms of the five carrier media in the terrestrial

	Phase	Unknown	Objective
1.	Screening study	f,X,k	Determine the subset X of important independent variables from the complete set of all potentially important independent variables.
	Empirical model building	f,k	Determine a suitable empirical representation of f along with associated values of k.
	Mechanistic model building	f,k	Determine the true functional form of f.
4.	Mechanistic model fitting	k	Determine the true value of ${\bf k}$ in the true form ${\bf f}$.

Table 2. Classification of Studies of the Model $Y = f(X,k)^*$

nitrogen cycle are listed in Table 3, along with a specification of their roles as influents, effluents, or internal carriers.

These media can also be thought of as the physical agents of the system. The presence of human agents in the system depends on the type of region under consideration. For example, an undisturbed wilderness forest would have no human agents, while in an agricultural system, human agents would serve as both consumers and manipulators.

The sequence element of the terrestrial nitrogen system consists of three types of processes—transportation by a carrier, exchanges between carriers, and transformations between different forms of nitrogen in a given carrier. A detailed qualitative study of the nitrogen cycle to identify these component processes has resulted in Table 4.

A proposed characterization of the environment for the terrestrial nitrogen cycle is presented in Figure 3. The upper boundary of the system is the top of the layer of animal and vegetative litter which rests on the surface of the soil. The lower boundary is the level of the groundwater table. The vertical direction is the only spatial dimension which will be considered at this time. It is assumed that lateral variations can be accounted for sufficiently by dividing a region to be modeled into homogeneous subregions within which areal variations are negligible.

While we propose to predict the concentration of nitrogen as a continuous function of depth, we realize that various parameters and variables of soils have not often been studied in this manner. Many earth

^{*}Taken from Hunter.5

Table 3. Functions of the Carrier Media in the Terrestrial Nitrogen Cycle

			Function		
Carrier	_		Input	Internal	Output
Water	1.	Precipitation	X		
	2.	Run-on	X		
	3.	Soil water		X	
	4.	Ground water	X		X
	5.	Water vapor		X	X
	6.	Runoff			Х
Fertilizer	7.	Organic fertilizer	X		
	8.	Inorganic fertilizer	Χ		
Organic	9.	Living organisms	X	X	X
matter	10.	Dead organic matter*	X		
Air	11.	Atmosphere	X		X
	12.	Soil air		X	
Soil	13.	Soil matrix		X	

^{*}Includes entire or parts of entire organisms and their metabolic wastes.

Table 4. Transportation, Exchange, and Transformation Processes in the Terrestrial Nitrogen Cycle

Transportations	Transformations
1. Gravity	1. Biological nitrogen fixation
2. Surface runoff and erosion	2. Ammonification
3. Infiltration	3. Immobilization
4. Redistribution	4. Nitrification
5. Diffusion and dispersion	5. Nitrate reduction
6. Capillary rise	6. Denitrification (chemical and
7. Faunalpedoturbation*	biological)
8. Translocation	7. Plant uptake
Exchanges	8. Excretion
1. Evaporation	9. Death
2. Dissolution	
3. Ion exchange and adsorption	
4. Ammonium fixation	

^{*}Movement of earthworms and other soil fauna as defined by Hole. 18

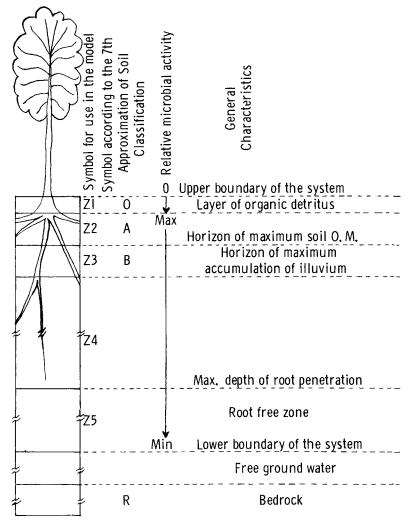


Figure 3. A proposed characterization of the environment for the terrestrial nitrogen system.

scientists have studied only selected regions of a soil system, e.g., topsoil, subsoil, root zone, or groundwater table. Therefore, to aid in obtaining data on the overall system from various researchers and from the literature, the soil system is divided conceptually into commonly-used horizontal layers for which some data are available. The criteria used to perform this division are spatial trends in the properties of a soil as viewed by a soil physicist, a soil chemist, and a pedologist. The latter scientist examines and classifies soils and soil profiles as they occur in the natural environment.

The first three zones of the profile in Figure 3, denoted as Z1, Z2, and Z3, correspond approximately to the O, A, and B horizons established by the 7th Approximation, Comprehensive Scheme of Soil Classification. The Z4 zone extends from the bottom of Z3 to the depth to which roots penetrate; the Z5 layer extends from this depth to the lower boundary of the entire system—the water table. The thickness of each of these five zones varies with the nature of the soil and vegetation being studied, and for some of the zones, e.g., Z1 and Z5, the thickness may also vary with time. This concept includes the possibility that at a given point in time in a given system, a zone might have zero thickness. It is recognized that unusual variations of soil and vegetation might necessitate modification of this zonation scheme, but we believe that this scheme is a good first approximation.

Ecosystems Under Investigation

Assuming that our systems approach is practicable, and that the system definition of the terrestrial nitrogen cycle is workable, then both should be applicable to most types of ecosystems. We are now conducting experiments to assess the validity of these assumptions by applying them to two ecosystems which can be imagined as being at opposite ends of a spectrum of man's intrusion in the affairs of nature. If this work succeeds, we will be reassured of the validity of this approach to systems intermediate to these two.

The first system is the Noe Woods, a micro-watershed in the University of Wisconsin Arboretum. This woods, primarily of black and white oak, is intended to represent an undisturbed, forested ecosystem. In accordance with the method illustrated in Figure 1, the system is being intensively monitored. The soil profile and litter layer of the Noe Woods are being sampled extensively at nine areas. Data are being accumulated on the spatial and temporal behavior of soil moisture contents, moisture tensions, temperatures, pH's, and nitrogen contents. The level of the groundwater table, surface runoff, air temperature, relative humidity, precipitation, evaporation, dust fall, and wind velocity are also being monitored in the immediate vicinity of the Noe Woods. These data will aid in inferring which processes listed in Table 4 are of primary importance, and in evaluating the validity of the system model at the end of the modeling study.

To provide the required sharp contrast to the undisturbed Noe Woods, the second ecosystem chosen for study is a set of field plots at the University of Wisconsin Agricultural Experiment Station at Hancock, Wisconsin. This system is highly manipulated to produce high yields of agronomic and truck crops by the use of supplemental irrigation, fertilizers,

and pesticides. The suction drainage and hydraulic weighing systems of the two field lysimeters installed at this site provide for convenient system monitoring.¹⁰ For several years, University scientists have acquired data on the physical properties and behavior of the sandy soil at this station, and of the nutrient uptake characteristics of the variety of irrigated crops grown in this region.¹¹

In some respects the dynamics of the Hancock system are simpler than those of the Noe Woods. The complex processes of litter fall and its subsequent decomposition are extremely important in the nitrogen dynamics of a forest soil, while in an agricultural system, litter fall and its incorporation by various cultivation practices can be controlled to alter its relative significance. The Z1 zone (Figure 3) of the Hancock model, therefore, will be smaller than that of the Noe Woods model. On the other hand, the Z5 of the Hancock model will be relatively larger than that in the Noe Woods model. This will be due to the shallowness of the roots, relative to the forested system, of most of the plants grown at the Hancock site, and to the irrigation and fertilization of the sandier soil.

System Model

The Law of Conservation of Mass provides a theoretical basis for developing a system mathematical model of the terrestrial nitrogen cycle. Imagine that at some depth z in the system there exists a volume element of soil. Nitrogen is traveling into and out of this volume element, as well as reacting within it. If mass is to be conserved within this element, the following relationship must be satisfied:

$${\text{Rate of Mass} \atop \text{Accumulation}} = {\text{Rate of} \atop \text{Mass In}} - {\text{Rate of} \atop \text{Mass Out}} + {\text{Net Rate of Appearance} \atop \text{of Mass by Reaction}}$$
(2)

Figure 4 portrays a volume element of unit cross-sectional area and length $\triangle z$. A fraction (ϵ) of this volume element is occupied by a carrier. The (cv) expression represents the transport in the z direction of a nitrogen compound at concentration c via the flow of a carrier medium with volumetric flux v, a type of process often referred to as convection or bulk flow. The infiltration and redistribution phenomena of the hydrologic cycle referred to in Table 4 are examples of convective processes. Since (cv) is a function of depth, its value at any z is denoted by $(cv)_z$. Nitrogen may also be transported by dispersive mechanisms, denoted in Figure 4 by the product of a dispersivity coefficient D and a concentration gradient $(\partial c/\partial z)$. Finally, the R_i term refers to the rate of a process in which a nitrogen species is being consumed, produced, or exchanged.

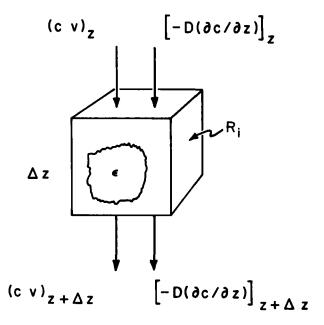


Figure 4. A theoretical volume element at depth z in the soil.

Equation 2 can now be written for the volume element of Figure 4 in a precise mathematical formulation known as the continuity equation (12):

$$\frac{\partial(\epsilon c)}{\partial t} = -\frac{\partial(cv)}{\partial z} + \frac{\partial}{\partial z} \left[\frac{\epsilon D(\partial c}{\partial z}) \right] / \frac{\partial z}{\partial z} + \sum R_i$$
 (3)

where: c = concentration of a nitrogen compound in a carrier (mass/unit volume of carrier)

 ϵ = volume of a carrier per unit volume of soil

v = volumetric flux of a carrier (volume of carrier/unit crosssectional area of soil/time)

D = dispersivity of a nitrogen compound in a carrier (cross-sectional area of carrier/time)

 R_i = a rate of reaction involving the nitrogen compound (mass/unit volume of soil/time)

t = time

z = depth

Using the previously described terminology of equation (1) and Table 2, c is a dependent variable, z and t are independent variables, and D is a parameter. The terms ϵ , ν , and R_i are dependent variables of the component processes of the system. Before equation (3) can be integrated to yield the response of c as a function of z and t, models which also

express ϵ , ν , and R_i as functions of z, t, and various parameters must be obtained. This requires process level studies in soil physics and soil chemistry, in a manner consistent with the scheme portrayed in Figure 1.

Dutt et al¹³ followed essentially the above plan to develop a mathematical model for predicting the nitrate content of agricultural drain water from an arid soil. The result was an excellent first approximation for a system model, of the type proposed in equation (3), of the terrestrial nitrogen cycle. We believe, however, that the use of the more sophisticated modeling and experimental techniques in the process studies proposed in the following sections can yield a still more refined simulation than that achieved by Dutt et al.

Process Studies in Soil Physics

The movement of water through soil can be described by Darcy's law, a one-dimensional form of which is:

$$v = -K(h) \, \partial(h - z)/\partial z \tag{4}$$

where: ν = volumetric flux in positive z direction (cm³ of water/cm² of soil/day)

K(h) = hydraulic conductivity (cm/day)

h = soil moisture pressure head (cm of water)

z = depth measured positive downward (cm)

When Darcy's law is substituted into the continuity equation for water, 14 the following dynamic equation results:

$$C(h) \frac{\partial h}{\partial t} = \frac{\partial \left[K(h)(\partial h/\partial z - 1)\right]}{\partial z}$$
 (5)

C(h), known as the specific moisture capacity (cm⁻¹), is actually the slope of the soil moisture characteristic curve, $\theta(h)$, which relates the soil moisture content $\theta(\text{cm}^3 \text{ water/cm}^3 \text{ soil})$ to the pressure head h. For the soil water regime, θ is analogous to the ϵ of equation (3).

A numerical integration of equation (5), which requires prior knowledge of the way in which C and K vary with h, i.e., C(h) and K(h), results in a dynamic profile of h vs z. This profile can be used in equation (4) to obtain a velocity profile for inclusion in equation (3). It can also be converted into a profile of θ if the moisture characteristic curve is known. It is the common practice of scientists investigating this problem to represent the functional relationships for $\theta(h)$, K(h), and C(h) in tabular form. Various interpolation schemes for these tables are then devised to produce a value of θ , K, or C for any given value of h. Our current process level studies are also directed toward developing models for producing

moisture content and velocity profiles to substitute into equation (3). We plan to accomplish this, however, by independent development of analytical expressions for $\theta(h)$ and K(h).

Because the $\theta(h)$ relationship is nonlinear and often hysteretic, its determination is a complex problem. Von Rooyen¹⁵ has provided field data on θ vs. h in each of the four horizons of the sand in the Hancock lysimeters. Using a nonlinear least squares algorithm, as explained in detail by Draper and Smith⁶, these data have been used to fit several nonlinear models in a search for the best equation for predicting the characteristic curve. Preliminary results from this modeling are very promising. Assuming that an adequate analytical representation of the moisture characteristic can be attained, the differentiation of this function will then yield the gradient $d\theta/dh$, i.e., the soil moisture capacity C(h).

Inasmuch as hydraulic conductivity measurements in the field are difficult to accomplish, values of K vs. h have been obtained partially from theory. Green and Corey¹⁶ recently reviewed the variety of modifications that have been made to a method for predicting the hydraulic conductivity of a porous medium based on pore-size distribution data. Since this distribution is actually manifested in the moisture characteristic, it is believed this method will dovetail conveniently with the efforts for modeling the moisture characteristic as described above. Preliminary results from the calculation and subsequent fitting of the generated K values to a nonlinear model in h are also encouraging.

Once analytical expressions for $\theta(h)$, K(h), and C(h) have been obtained, they will be included in an algorithm to numerically solve equations (5) and (4). The logic of this algorithm and the skeleton of a computer program for implementing it have already been devised. Once this model is built, it will be evaluated using data obtained from moisture flow experiments on the Hancock lysimeters. In accordance with the scheme for systems analysis illustrated in Figure 1, this initial testing of the overall model will lead to a modification of it and subsequent re-evaluation. Several iterations will be required before a final evaluation of the results and accuracy of the simulation can be made. If this work proves successful, a foundation will have been laid for achieving an analagous predictive capability on natural, more complex ecosystems, such as the Noe Woods, using similar experimental and modeling techniques.

Process Studies in Soil Chemistry

A list of the biochemical transformations in which soil nitrogen is involved was introduced in Table 4. Reaction equations for each of these are presented in Table 5 using convenient abbreviation symbols for the six

Table 5. Soil Nitrogen Transformations

Nitrogen species to be accounted for	Shorthand symbol	Symbolic reaction equations		
1. NH ₄ - Ammonium ion	NH4	 Biological nitrogen fixation NGF→NLO 		
2. NO ₂ - Nitrite ion	NO2	2. Ammonification NDO→NH4		
3. NO ₃ - Nitrate ion	NO3	 Immobilization NH4→NLO; NO2→NLO; NO3→NLO 		
4. N bound in living organic matter	NLO	4. Nitrification NH4→NO2→NO ₃		
5. N bound in dead organic matter	NDO	 Nitrate reduction NO3→NO2→NH4 		
6. N bound in gaseous form	NGF	6. Biological denitrification NO3→NO2→NGF		
		 Chemical denitrification NO2→NGF 		
		8. Plant uptake NH4→NLO; NO2→NLO; NO3→NLO		
		9. Excretion NLO→NDO		
		10. Death NLO→NDO		

nitrogen species to be accounted for in the study. The first three of these species are common inorganic ions of nitrogen. The last three are not unique molecular compounds of nitrogen, but rather an aggregate of nitrogen containing substances with common characteristics. This characterization was thought to be a good compromise between the need to account for these obviously important forms of nitrogen, and the impracticability of distinguishing among the many unique compounds which constitute each of the three groups.

The objective of the proposed process studies in soil chemistry is the development of an analytical expression for the rate of each reaction in Table 5. These rates will be a function of independent variables such as temperature and moisture content, of parameters such as rate constants and metabolic efficiencies, and of dependent variables such as the concentrations of the nitrogen species themselves. While the modeling study of all these reactions will follow the pattern outlined in Table 2, in light of the differences in complexity between the transformations, not all the studies

are expected to result in models of equal sophistication. The model of nitrogen immobilization, for example, may be no more than an empirical model based on linear regression of literature data, e.g.,

$$-d(NH4)/dt = a_0 + a_1(NH4) + a_2(NLO) + a_3T + a_4\theta$$
 (6)

where: () = concentration of nitrogen species

 a_i = regression coefficient

T = temperature

The kinetics of nitrification, on the other hand, may be studied theoretically and experimentally, resulting in nonlinear models such as:

$$-d(NH4)/dt = a_1 \left[\exp(-a_2/T) \right] (NH4)a_3 (NO3)a_4$$
 (7)

McLaren¹⁷ has proposed several Michaelis-Menten type equations which could also serve as potential mechanistic models for nitrification.

A preference for developing mechanistic models has motivated our initial process studies in soil chemistry. We are conducting a screening study (see Table 2), using a two-level factorial design, to determine the magnitude of the main and interaction effects of four variables on the overall nitrogen dynamics in undisturbed cores extracted from different horizons of the Noe Woods soil profile. The levels of these four variables—temperature, moisture content, concentration of ammonium ion, and of nitrate ion—will be evaluated periodically while the cores incubate for several weeks. As in our soil physics studies, nonlinear least squares theory will then be used to estimate the parameters in the proposed rate models. Based on analyses of the results of these experiments, further studies will be made of the kinetics of individual reactions, and of the mechanistic roles of these, and possibly other, independent variables.

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