This workshop was sponsored by
IUBS (International Union of Biological Sciences), Paris
SCOPE (Scientific Committee on Problems of Environment) of the
ICSU (International Council of Scientific Unions), Paris
Ministry of Agriculture and Fisheries, The Hague

Simulation of nitrogen behaviour of soil-plant systems

Papers of a workshop
Models for the behaviour
of nitrogen in soil
and uptake by plant.
Comparison between
different approaches
Wageningen, the Netherlands
January 28-February 1, 1980

Editors: M.J. Frissel and J.A. van Veen

1981
Centre for Agricultural Publishing and Documentation
Wageningen

ISBN 90-220-0735-9

Printed in the Netherlands

Contents

1. Introduction

D.J. Greenwood

Crop yields throughout the world are often severely restricted by lack of nitrogen. This results partly from the high cost of increasing nitrogen levels in soil and partly from the difficulty in forecasting how to adjust N fertilizer levels for differences in crops and soils. In some areas too much nitrogen may be applied as fertilizer or as organic manures and when this happens both yields and crop quality can be severely depressed and the concentration of nitrate in the drainage water may rise sufficiently to cause public concern. Thus, agronomic practices that influence the nitrogen status of soil have both merits and limitations. Although much is known in qualitative terms about the nitrogen cycle there is still no satisfactory way of choosing the best practice for any particular set of conditions.

The most favoured approach relies on carrying out field experiments on the soils where the information is most needed. Undoubtedly, considerable progress has been made in this way but there are, nevertheless, serious difficulties. These stem form the critical dependence of the results of such experiments on the weather conditions and the impracticability of carrying out experiments that cover more than a few of the possible combinations of crop, soil and weather. It is, therefore, necessary to extrapolate from the results to a wider range of conditions which inevitably leads to much error and inadequate advice on the choice of practice.

Much basic work has been carried out on the most important processes affecting the levels of inorganic nitrogen in soil, and their influence on crop nitrogen nutrition and growth. Considerable attention has been given to mineralization and immobilization, transport of water and inorganic nitrogen through soil and the mechanism of ion adsorption by plant roots. The main processes are well understood in qualitative terms and models based on this understanding have been devised for the day-to-day changes in soil nitrogen status and in plant growth. Some of the models are aids to understanding, whilst others aim to predict the benefits of different practices in various situations. Their development is of much interest in many parts of the world.

Progress in the subject is undoubtedly hindered by difficulties in communication. Models span many disciplines, are often complex, inherently difficult to understand and are seldom described in the scientific literature in sufficient detail to be helpful to other workers. The net result is that there are a range of apparently different models purporting to do the same thing. Some of the discrepancies may result from different concepts for individual processes. But whatever the cause there is much misunderstanding and need for discussion.

It is, therefore, very timely that the soil-plant group at ITAL with the support of IUBS and SCOPE, should organize a small international meeting of scientists who have modelled different aspects of the nitrogen cycle. The meeting was held in the Institute of the ITAL Foundation, Wageningen, The Netherlands) from 28 January until 1 February 1980.

The first two days were spent in open sessions with all participants listening to oral presentations of the models (working papers had been presented previously) and discussing them in depth. Separate groups then discussed classification and soil physical, soil microbial and plant physiological aspects of the various models. In these the "state of art" was reviewed and the factors limiting progress identified.

The book brings together the results of this work. There is a chapter describing the reports of the four groups, another summarizing the features of the models and others describing each of the models in greater detail. It is hoped that this presentation will help the reader appreciate the purposes, merits and shortcomings of the various approaches to the simulation of nitrogen behaviour in soils and plants and will help him judge the opportunities for advance.

2. Systematic comparison of the models described

M.J. Frissel, G.J. Kolenbrander, I. Shvytov and O.F. Vasiliev

The aims of the models considered in this publication vary widely. Some models concentrate on a particular process, for instance on leaching or on losses by denitrification. Other models try to cover a very wide field, but these models also differ considerably in their underlying concepts, mainly because of differences in the significance attributed to the role of soil organic matter and of water regime.

Table 1 indicates whether a certain process is included in a particular model or not. The table does not provide information on the degree of sophistication. For instance, mineralization/immobilization may be described by one single first-order equation or by a whole set of equations. In either case the table simply indicates that mineralization/immobilization is included in the model. Models which are based on similar concepts are grouped together to improve readability. The first five models (section 4.1 - 4.5) are the most general ones: the microbiological processes are described by rather simple equations. The next four models (sections 4.6 - 4.9) take particular account of the role of microorganisms in mineralization/immobilization. The models described in sections 4.9 and 4.10 give special attention to dry matter production. The model of section 4.11 concentrates on long term prediction, and each of the last four models on one process only: volatilization, leaching or denitrification.

There are other differences between the models. Some of them have been developed for better understanding of the processes while others concentrate on prediction of available mineral N or on overall management. These differences are indicated in Table 2. It is realized that this division is rather arbitrary. Well developed 'better understanding models' can for instance give results useful for 'management purposes', but the amount of input data is often so large that this is impracticable.

Table 2 also provides information on the period for which the model is intended and on the type of equations. This division is again arbitrary. Both the partial differential equations and normal differential equations are often replaced in a computer program by simple difference equations, so that the contrast between the various types of equations vanishes.

This section also contains a short description of each model, all in a similar format. Several models are included which were not presented at the workshop, but which were analysed by Shvytov and Vasiliev for this workshop.

Table 1. Main characteristics of the models.

Processes	Models	Tanji, Mehran, Gupta	Wagenet	Rao, Davidson, Jessup	Selim, Iskandar	Kruh, Segall	Van Veen, Frissel	Juma, Voroney, Paul	Bosatta	McGill, Hunt, Woodmansee, Reuss, Paustian	Seligman, Van Keulen	Russell	Parton, Gould, Adamson, Torbit, Woodmansee	Addiscott	Leffelaar	Smith
	described in section	4.1	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	4.10	4.11	4.12	4.13	4.14	4.15
Microbiological	urea → NH_4		x										x			
	miner./immob.	x		x		x	x	x	x	x	x	x		x		
	microb. biomass						x	x	x	x						
	nitrific.	x	x	x	x	x	x			x						
	denitrific.	x	x	x	x	x	x			x						x
	biol. N_2-fix									x						
Plantphysiol.	water uptake	x	x	x	x	x				x	x			x	x	
	dry matter prod.		x							x	x	x				
	root growth	x	x	x						x	x					
	debris, exudation									x						
	N uptake	x	x	x	x	x			x	x	x			x		
Physical	waterflux	x	x	x	x	x	1)		1)	1)	x		x	x	x	
	heatflux		x			x	1)									
	gasflux					x							x		x	
	NH_4 ads./exch.	x	x	x	x		x		x	x			x			
	NH_4-volatil.		x				x				x		x			
	leaching	x	x	x	x	x	x		x	x	x			x		

[1] data on waterflux and moisture content and/or heat flux are derived from an other (external) simulation program.

Table 2. Additional characteristics of the models.

Characteristics	Models	Tanji, Mehran, Gupta	Wagenet	Rao, Davidson, Jessup	Selim, Iskandar	Kruh, Segall	Van Veen, Frissel	Juma Voroney, Paul	Bosatta	McGill, Hunt, Woodmansee, Reuss Pausian	Seligman, Van Keulen	Russell	Parton, Gould, Adamson, Torbit, Woodmansee	Addiscott	Leffelaar	Smith
	described in section	4.1	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	4.10	4.11	4.12	4.13	4.14	4.15
main objective	scientific understanding	x	x		x		x	x	x	x			x		x	x
	forecast					x						x		x		
	management			x							x					
time horizont	days	x			x								x		x	x
	months		x	x	x	x	x	x	x	x	x			x		
	years						1)			x		x				
input data	climatic	x	x	x	x	x	x		x	x	x		x	x	x	
	soilphysical	x	x	x	x	x	x		x	x	x		x	x	x	x
	soil bio-chemical	x	x	x	x	x	x	x	x	x	x	x				x
	soil micro-biological						x	x	x	x						
	vertical distribution of parameters	x	x	x	x	x	x			x	x			x		x
type of equations	partial differential	x	x		x	x							x		x	
	differential		x	x	x	x	x	x	x	x		x				x
	balance			x					x		x	x	x	x		x

---

1) A very long term version of the model exists, but is not included.

K.K. Tanji, M. Mehran, S.K. Gupta
Water and nitrogen fluxes in the root zone of irrigated maize (section 4.1.)

Processes

Physical processes: water movement in the soil in vertical direction, NH_4^+ adsorption, exchange, NH_3 volatilization, nitrogen leaching. N uptake by plants is considered.
Microbiological processes: mineralization, immobilization, denitrification.

Techniques

Time horizon is several months. Partial differential equations are used. Finite difference approximation is applied.

Input

Water flow submodel: climatic data, number and depth of segments of soil, dates of planting and harvesting, hydraulic conductivity.
Other sub-blocks of model need soil-physical and biochemical data.

Output

Dynamics of water content in the soil profile, dynamics of different nitrogen species in the soil profile and amount of nitrogen leached.

Additional remarks

One of the main objectives is to simulate different irrigation schedules and leaching patterns.

R.J. Wagenet
Simulation of soil-water and nitrogen movement (section 4.2.)

Processes

Physical processes: water movement and leaching in soil in vertical direction, heatflux, NH_4^+ adsorption, exchange and fixation. Ammonia volatilization. Water consumption by plants is considered.
Biological processes: denitrification, hydrolysis of urea and nitrification.

Techniques

Partial differential equations are used. Finite difference approximation is applied. Three first-order kinetic differential equations are used to describe the chain of nitrogen transformations in the soil.

Input

Soil physical and bio-chemical data are required as well as data on rainfall and other climatic data.

Output

Main output is soil-water pressure head, volumetric water contents, nitrogen species concentrations and nitrogen uptake by plants.

Additional remarks

On the main objectives is to simulate N leaching and uptake by plants after application of urea. Irrigation is included.

P.S.C. Rao, J.M. Davidson and R.E. Jessup
Simulation of nitrogen behaviour in the root zone of cropped land areas receiving organic wastes (section 4.3.)

Processes

Physical processes: vertical water flux and redistribution of water, NH_4^+ adsorption and exchange, leaching.
Microbiological processes: mineralization, immobilization, nitrification and denitrification. Water and nitrogen uptake by the crop are considered.

Techniques

Finite difference equations are used to model water movement and solute transport in the soil. Balance empirical relations are used to describe water and nitrogen uptake by plants. Nitrogen transformations are described by linear differential equations.

Input

Main input: climatic data and soil physical and bio-chemical data. Manure and nitrogen fertilizer application is also required as input.

Output

Dynamics of different forms of soil nitrogen. Water content in the soil profile and water outflow, gaseous nitrogen losses and organic carbon content are calculated.

Additional remarks

Main objectives are simulation of nitrogen behaviour in soil and its uptake by crops after application of fertilizer, animal manure or plant residues.

H.M. Selim and I.K. Iskandar
A model for nitrogen behaviour in soils irrigated with liquid waste (section 4.4.)

Processes

Physical processes: vertical water flux, NH_4^+ adsorption, exchange, leaching is included. Water and nitrogen uptake by plants is considered.
Microbiological processes: nitrification and denitrification.

Techniques

Partial differential equations for ammonium, nitrate, and water transport in soil. Nitrogen uptake is calculated by simple equations as function of root density and N-concentration in soil.

Input

Main input: wastewater application. Soil physical and bio-chemical data are required, rate of N uptake by plants.

Output

Dynamics of water content in the soil profile, dynamics of different nitrogen species in the soil profile, amount of nitrogen leached, plant uptake of N.

Additional remarks

The model can be used to study the fate of fertilizer nitrogen applied to agriculture land.

G. Kruh and E. Segall
Nitrogen dynamics in soil (section 4.5.)

Processes

Physical processes: vertical water flux, heat and gas flux; leaching can be calculated. Water and nitrogen uptake are included.

Microbiological processes: mineralization, immobilization, nitrification and denitrification.

Techniques

The time horizon for this model is several months. Modelling of water flow is based on an extended Darcy equation. Vertical flow of oxygen through the soil is modeled by Fick's equation.

The rate of nitrification is approximated by a parabolic function of time. Denitrification is described by modified first order kinetics.

Input

Main input: climatic data, soil physical and soil bio-chemical data. Many empirical correlation factors are required.

Output

Main output: dynamics of soil water content, concentration of ammonia and nitrate in soil, water and nitrate outflow.

Additional remarks

The model can be implemented to calculate nitrogen leaching from root zone of cropland. Further, the model can be used to estimate nitrogen fertilizer requirements under various conditions.

J.A. van Veen and M.J. Frissel
Simulation model on the behaviour of N in soil (section 4.6.)

Processes

Microbiological processes: mineralization, immobilization, microbial growth and death, nitrification and denitrification. The physical processes used are ammonium adsorption and exchange and NH_3-volatilization. Leaching can be calculated.

Techniques

Zero-order rate kinetics, first-order rate kinetics, Monod kinetics. The soil organic carbon is divided into 6 pools. For all processes, except denitrification, a multilayer approach is used. The denitrification model considers sets of concentric peels to calculate the oxygen diffusion. Anaerobic conditions occur at locations where oxygen consumption is higher than the supply of oxygen by diffusion. The link between the denitrification program and other parts of the program is poor.

Input

The main driving variables are manure, fresh organic matter and nitrogen fertilizers application. Numerous other data are required. Some of these, as e.g. microbiological data are difficult to measure. Optional values are available. Heat- and water-flux description are derived from the model of Beek and Frissel, 1973.

Output

Ammonium, nitrite and nitrate concentrations in the soil, microbial biomass, denitrification and volatilization losses of nitrogen, leaching of nitrates.

Additional remarks

This model is designed to improve understanding of the nitrogen transformation processes in the soil. It enables simulating various microbiological scenarios under different natural and technological conditions. A program version which enables following the fate of ^{15}N within the soil organic matter is available.

N.G. Juma, R.P. Voroney and E.A. Paul
Use of tracers and computer simulation techniques to assess mineralization and immobilization of soil nitrogen (section 4.7.)

Processes

The change in biomass in relation to mineralization and immobilization is considered in detail.

Techniques

Zero-order rate kinetics and first-order rate kinetics. The soil organic carbon is divided into 7 pools, each having its own availability as substrate for microorganisms.

Input

The main driving variables are manure, fresh organic matter and nitrogen fertilizers.

Output

Ammonium concentration, N and C-content of different soil organic matter pools.

Additional remarks

The model can be used to obtain a better understanding of the nitrogen transformations in soil. A program version which enables following the fate of ^{15}N and ^{14}C, besides ^{14}N and ^{12}C within the soil organic matter is available.

E. Bosatta
Plant soil system of an old Scots Pine forest in Central Sweden (section 4.8.)

Processes

Microbiological processes: mineralization, immobilization.
Physical processes: ammonium adsorption and exchange. Leaching can be calculated. All mineral nitrogen is assumed to be ammonium. Nitrogen uptake by plants is included.

Techniques

All processes are described by differential equations. The decomposition processes are carbon and/or nitrogen limited, the C/N quotient is an important variable. N_2-fixation and incorporation of N into biomass is considered, adsorption and desorption of ammonium is instananeous. Uptake by roots is controlled by root geometry, diffusion of ammonium and ammonium concentration.

Input

Soil temperature, water content and water flow are derived from another program (not described here). Microbiological data such as biomass production and mortality rates are required. Driving variables are forest litter production and nitrogen in rain. Data are required to split the litter in C-C and C-N compounds.

Output

Biomass, C-C and C-N compounds in soil. A verifiable parameter is the NH_4 concentration.

Additional remarks

The model considers trees. Verification of this model of a forest ecosystem is significantly more difficult than of a model which describes a crop-system. The growth season (April-November) of four different years was simulated.

W.B. McGill, H.W. Hunt, R.W. Woodmansee, J.O. Reuss and K.H. Paustian
Formulation, process controls, parameters and performance of PHOENIX: A model of carbon and nitrogen dynamics in grassland soils (section 4.9.)

Processes

Microbiological processes: mineralization-immobilization. Two decomposer groups are considered: bacteria/actinomycetes and fungi. Nitrification (with inhibition), denitrification.
Plantphysiological processes: ammonium uptake, nitrogen uptake, senescence and death.
Physical processes: application fertilizers, leaching.

Techniques

Finite difference equations. Very extended model, therefore most equations rather simple.

Input

One of the most extended models, therefore many input parameters.

Output

Mineral soil nitrogen, dry matter production. Soil micro-organisms. CO_2 production.

Additional remarks

Objective: exploration, through simulation modeling, the relationships among plant processes and microbial processes and their effect on plant production, microbial secondary production and N-cycling. Emphasis on microbes, soil organic matter and mineral N.

N.G. Seligman and H. van Keulen
PAPRAN: A simulation model of annual pasture production limited by rainfall and nitrogen supply (section 4.10.)

Processes

Microbiological processes: mineralization, immobilization.
Plant physiological processes: root growth, dry matter production, water and nitrogen uptake by crops.
Physical processes: vertical water-flux and ammonium volatilization. Leaching can be calculated.

Techniques

The time horizon is one (Israelian) growing season. The growth of the plant is calculated by difference equation. Driving force is solar radiation. Water and nitrogen limit the dry matter production. Water and nitrogen transport through soil are described as supply and demand balances. Nitrogen transformations in the soil are modeled as balance processes dependent on soil physical and biochemical factors.

Input

Climatic, soil physical and biochemical data are required.

Output

Dynamics of dry matter production, nitrogen content in various plant organs, soil moisture content, mineral-N in soil, organic-N in soil.

Additional remarks

Main objective is to generate data on dry matter production function of water and mineral nitrogen availability as a means for management decisions (semi-arid grasslands).

J.S. Russell
Models of long term soil organic nitrogen change (section 4.11.)

Processes

Microbiological processes: mineralization, immobilization. Dry matter production of crops is included.

Techniques

Time horizon: several decades. Linear differential equations solved numerically.

Input

Plant yield data and soil bio-chemical data.

Output

Dynamics of mineral nitrogen in the soil and plant yield.

Additional remarks

The model can be used for long term predictions of the organic-N content of soils.

W.J. Parton, W.D. Gould, F.J. Adamsen, S. Torbit and R.G. Woodmansee
NH_3-volatilization model (section 4.12.)

Processes

Physical processes: gas-flux, ammonium adsorption and -exchange, ammonium volatilization. Hydrolysis of urea.

Techniques

Difference equation based on Michaelis-Menten kinetics diffusion equation. For several steps instantaneous equilibrium is assumed. Partial differential equation to describe water flow.

Input

Soil physical and bio-chemical data.

Output

Data on hydrolysis of urea, NH_3-volatilization, water flow and leaching.

Additional remarks

Main objective is to quantify losses of volatile NH_3 as function of environmental conditions.

T.M. Addiscott
Leaching of nitrate in structured soils (section 4.13.)

Processes

Leaching, calculated from the vertical water-flux, making allowance for mobile and retained waterphases.
Mineralization (optional).

Techniques

A multi-layer approach is used. During water flow, only nitrate in the mobile phase is displaced, with nitrate in the retained phase held back. When water flow ceases, nitrate transfer between the phases may occur instantaneously or by diffusion. Mineralization is proportional to the square root of time.

Input

Rainfall, evaporation. Points on the soil moisture characteristic *or* aggregate size distribution and porosiby. Nitrate inputs from fertilizer and rain. Constant relating mineralization to the square root of time, and its relation to temperature (optional).

Output

Nitrate concentration in profile and leachates (drainage water).

Additional remarks

Main goal is to obtain understanding of the influence of soil aggregates on leaching and to investigate how solutes held in soil aggregates may be protected from leaching. The model can connect leaching with either the water retention characteristics of the soil or with the mechanical characteristics of aggregation and porosity.

P. Leffelaar
Model to simulate partial anaerobiosis (section 4.14.)

Processes

Physical processes of water- and gas-flux.

Techniques

Use of detailed geometrical models, difference equations.

Input

Soil physical data and oxygen consumption rate.

Output

Oxygen concentration in soil as function of environmental conditions.

Additional remarks

The model can be used to predict anaerobiosis.

K.A. Smith
A model of denitrification in aggregated soils (section 4.15.)

Processes

Denitrification.

Techniques

Equilibrium model. Differential equations for diffusion within aggregates and down into the soil profiles. Equations are analytically solved by assuming certain steady state cases.

Input

Parameters for describing the soil aggregates, physical constants to describe oxygen diffusion, oxygen-consumption rate of soil, concentrations and coefficients for nitrate and the gaseous products of denitrification.

Output

Fraction of soil which is anaerobic, denitrification rate.

Additional remarks

The model can be helpful in calculating denitrification. The model has not yet been tested.

I.G. Burns, 1975
An equation to predict the leaching of surface-applied nitrate. Journal of Agricultural Science, Cambridge, 85: 443-454. (Not presented at workshop.)

Processes

Water and nitrate movement through soil. Nitrogen transformation processes are not considered.

Techniques

The model assumes that rainfall will increase the water content of any soil layer until its field capacity is reached. The fraction of nitrate leached is correlated with fraction of water percolated.

The amount of nitrate leached below root zone is calculated, assuming that the soil solution of each layer is an equilibrium with water percolated.

Input

Water drainage through the soil.

Output

The fraction of surface-applied nitrate leached below any depth.

Additional remarks

Main goal is calculating nitrate leaching under rainfall and irrigation conditions for a wide range of fallow or cropped soil. The model might be a useful submodel in someone else's model.

J. Duffy, C. Chung, C. Boast and M. Franklin, 1975
A simulation model of biophysiochemical transformations of nitrogen in tile-drained corn belt soil. Journal of Environmental Quality, 4: 477-486. (Not presented at workshop.)

Processes

Water movement: unsaturated flow, saturated flow, water table fluctuations, tile flow of water.
Nitrogen transformations and movement processes: nitrification, mineralization, immobilization, denitrification, nitrate vertical movement, nitrate tile flow.
Crop growth: root growth, plant growth, nitrogen uptake.

Techniques

Vertical multi-layer model. Water flow rate between levels is calculated according to Darcy's equations. Zero and first-order reactions are used to model nitrogen transformation processes. Soil moisture, temperature, nitrogen and light are taken into account through Liebig's 'Law of Minimum Factors'.

Input

Main inputs are nitrogen fertilizers and rainfall.

Output

Main outputs are the amount of water leaving the field as drain-tile effluent and nitrate concentration in tile effluent.

Additional remarks

The model is applicable to any typical field in the Corn Belt. It is possible to predict nitrate concentrations in the tile effluent as a function of farm management and climatic conditions.

M.H. Frere, M.E. Jensen and J.N. Carter, 1970.
Modelling water and nitrogen behaviour in the soil-plant system. Proceedings Summer Computer Simulation Conference: p. 746-760. (Not presented at workshop.)

Processes

Water balance processes: evapotranspiration, drainage.

Nitrogen balance processes: nitrification, mineralization, ammonification. Plant growth.

Techniques

Zero-order and first-order rate kinetics. Water balance modelling technique assumes that hydraulic gradient during drainage is independent of evapotranspiration. Accumulated dry matter during growing season follows an S-shaped curve. The rooting depth increase follows the equation for normal distribution.

Input

Daily climatic conditions (rain, minimum and maximum temperature, solar radiation, dew-point temperature, windspeed), irrigation water, nitrogen fertilizer.

Output

Nitrogen concentration in soil, soil water content, dry matter of crop, nitrogen leaching from root zone of soil.

Additional remarks

Main goal is to obtain a better understanding of the behaviour of water and nitrogen in the soil-plant system.

H. Laudelout, L. Germain, P.F. Chabalier and C.N. Chiang, 1977.
Computer simulation of loss of fertilizer nitrogen through chemical decomposition of nitrite. Journal of Soil Science, 28: 329-339. (Not presented at workshop.)

Processes

Ammonification, oxidation of ammonium in soil and chemical decomposition of nitrite. Water balance processes are not considered.

Techniques

First- and second-order rate kinetics are used. Competing microbiological systems are considered.

Input

Main input is nitrogen supplies.

Output

Concentrations of the nitrogenous species in the soil and nitrogen losses due to chemical decomposition of nitrite.

Additional remarks

Main goal is prediction of the rate of nitrogen loss from soil as a result of chemical decomposition of nitrite. The model promotes understanding the role of two competing reactions in which nitrite is biologically oxidized to nitrate or is chemically decomposed at low pH.

J.O. Reuss and G.C. Innis, 1977
A grassland nitrogen flow simulation model. Ecology 58: 379-388. (Not presented at the workshop.)

Processes

Mineralization of soil organic nitrogen, oxidation of ammonium to nitrate, nitrogen uptake by live roots, the transfer of nitrogen from the live top to the litter, the transfer of litter nitrogen to soil organic matter, immobilization of nitrogen during decomposition of roots, root growth processes. Effects of temperature and soil water availability on the various processes.

Techniques

Multi-layer model. All nitrogen flows are described as a function of time, soil temperature, soil water content, nitrogen content, plant growth. Nitrogen uptake by roots is sum of two processes, each of which is described by Michaelis-Menten relationships.

Input

Soil water and temperature data are required. Initial levels of different nitrogen forms in the soil.

Output

Plant biomass production and various nitrogen concentrations.

Additional remarks

Main goal is to obtain a better understanding of grassland ecosystem processes and fertilizer effects on grassland ecosystem.

K.E. Saxton, G.E. Schuman and R.E. Burwell, 1977
Modelling nitrate movement and dissipation in fertilized soils. Soil Science Society of America Journal, 41: 265-271. (Not presented at workshop.)

Processes

The vertical water and nitrate ion movement in the soil; plant uptake of nitrogen; nitrification, mineralization.

Techniques

Multi-layer model. Soil moisture - tension - conductivity relationships are used to describe vertical moisture movement. Nitrogen uptake from each soil layer is proportional to both the water uptake and the nitrate concentration of the water in the layer. The production of nitrate from applied ammonium fertilizer is uniform in the upper 15 cm layer.

Input

Precipitation and runoff; pan evaporation; plant canopy development; nitrogen fertilizer application.

Output

Dynamics of nitrate movement.

Additional remarks

Main goal is to obtain a better understanding of how to maintain optimum nitrate in the soil for crop use and to minimize potential environment pollution. The model can be applied to agricultural watersheds with permeable soils and high-yielding corn.

M.J. Schaffer, G.R. Dutt and W.J. Moore, 1969
Predicting changes in nitrogenous compounds in soil-water systems. Water Pollution Control Research Series. 13030 ELY, pp. 15-28. (Not presented at workshop.)

Processes

Mineralization, immobilization (both ammonia and nitrate), nitrification, urea hydrolysis. Water balance not considered.

Techniques

Transformation rates are a function of urea concentration, NH_3, organic-N, NO_3, C/N ratio, pH, temperature, moisture. A computerized multiple linear regression technique was applied.

Input

Initial soil conditions and nitrogen additions (urea, ammonia, organic-N, nitrate).

Output

Concentrations of the nitrogenous species in the soil with time.

Additional remarks

The model can be considered as a potential submodel for an integrated simulation model of nitrogen leaching after combining with a water balance model.

B. Singh, C.R. Biswas and G.S. Sekhon, 1978
A rational approach for optimizing application rates of fertilizer nitrogen to reduce potential nitrate pollution of natural water. Agricultural and Environment, 4: 57-64.
(Not presented at workshop.)

Processes

Nitrogen fertilizer application, nitrogen uptake by plants, nitrogen leaching.

Techniques

Steady-state model; grain yield and nitrogen uptake uptake for wheat and corn are described as a quadratic response function of nitrogen fertilizer applied.

Input

Quadratic response functions.

Output

Relations between fertilizer applications, economic returns and nitrogen losses.

Additional remarks

Main goal is optimalization of fertilizer application with respect to economic returns and permissible nitrogen releases.

K.K. Tanji, M. Fried and R.M. van de Pol, 1977
A steady-state conceptual nitrogenmodel for estimating nitrogen emissions from cropped lands. Journal Environmental Quality, 6: 155-159. (Not presented at workshop.)

Processes

- Hydrologic submodel: irrigation water flow, precipitation, water inflow to root zone, water outflow from root zone, evapotranspiration, surface return flow, seep percolation.
- Nitrogen submodel: irrigation water nitrogen inflow, precipitation nitrogen inflow, nitrogen fertilization, denitrification, nitrogen consumption by crops, nitrogen leaching.

Techniques

Model is based on two principles: steady state and mass balance. It has an annual or growing season time scale.

Input

N in irrigation water, N in precipitation, applied fertilizer, N_2 fixation, irrigation water-flux, precipitation.

Output

Main output data:
- quantity of deep percolated water;
- nitrogen leaching losses.

Additional remarks

Main goal is prediction of nitrogen leaching losses on croplands under intensive production, located in humid regions or where irrigation has been practiced for a long period.

M.F. Walter, G.D. Bubenzer and J.C. Converse, 1975
Predicting vertical movement of manurial nitrogen in soil. Transactions of the ASAE, 18: 100-105. (Not presented at workshop.)

Processes

Microbiological reactions: mineralization and nitrification.

Water balance processes: infiltration, percolation, drainage. Nitrate dispersion due to mass flow of soil solution. Vegetation is not considered.

Techniques

Zero-order kinetics were used to model nitrogen transformation processes. The one-dimensional unsaturated flow equation was applied to model water movement.

Input

Main input is manure application.

Output

Dynamics of nitrate concentrations in soil.

Additional remarks

Main aim is predicting nitrogen transformations and movement in the soil. It can be applied to lands with heavy applications of livestock waste in early spring.

3. Status report on modelling of the processes

3.1 Migration processes in soils

T.M. Addiscott, J.M. Davidson, K. Harmsen, P.A. Leffelaar, W.J. Parton, P.S.C. Rao,
J.H. Rayner, K.A. Smith, R.J. Wagenet[1]

In general, it appears that our mathematical skills exceed our knowledge about the biological system being described and the quality of input data available. Thus, care should be taken when evaluating output from nitrogen models based on minimal knowledge and inadequate input data.

WATER MOVEMENT

The physical processes responsible for the movement of water through weakly-structured, non-swelling soils are understood sufficiently well to justify the use of mechanistic-type models (Tanji, Wagenet, Selim, Iskander, Davidson et al.). However, these models are not well suited for describing the entry and redistribution of water into well-structured soils containing cracks or exceptionally large macropores that conduct water at much larger rates than those in the surrounding porous medium. Soils of the latter type have only recently been considered in sufficient detail, and a limited number of conceptual models have been developed to describe the phenomenon (Addiscott, Leffelaar, Smith, Van der Ploeg, Bouma). Input to drive these models generally involves bulk density, soil-water characteristic data and aggregate size distribution (dry sieving).

Input data for the deterministic models should be obtained from in situ measurements when possible, or from undisturbed soil cores. A sufficient number of measurements should be made to provide an estimate of the precision of each parameter or coefficient used. Also, as far as possible, the precision associated with each input value should be kept approximately equal. This, however, is frequently not possible owing to the spatial variability of field soils and frequency distributions associated with specific soil property measurements. For example, measurements of soil capacity terms (bulk density, soil-water content, tension at a specific soil depth, sand, silt and clay contents) are usually normally distributed, whereas intensity parameters associated with rate processes (hydraulic conductivity, diffusivity and soil-water-flux) exhibit non-normal (ususally log-normal) distributions. Thus, only a few samples are needed to describe the capacity parameters, but several orders of magnitude more samples are needed to describe rate coefficients with equal precision. This presents a serious problem to the modeler because cost and time considerations usually prevent him or her from achieving the same level of

[1] Alphabetical order.

precision for all model input parameters. The precision of the soil-water transport model will, in general, be established by the rate-determining parameters used to drive these models.

The resolution of most soil-water models should not be assumed to be better than that which the parameters represent. For example, if the input parameters are measured at depth intervals of 15 to 30 cm, the model should not be expected to quantify variations occurring within a 5 cm depth with equal or greater precision than those between 15-30 cm intervals.

Empirical models for describing soil-water movement using only capacity terms such as maximum soil-water content and field capacity may be a reasonable compromise to the problems associated with spatial variability of rate process coefficients (Rao, Davidson, Jessup, Addiscott). These types of technique are especially well suited for making management-type decisions or for general forecasting. They also provide a sufficient amount of output information to drive a solute transport model while requiring a minimum number of basic, but readily available, input parameters.

SOLUTE MOVEMENT (NO_3 AND NH_4)

The description of non-adsorbed solutes (Cl^- and NO_3^-) through weakly-structured, non-swelling soils can be described reasonably well with input from mechanistic or physically-based soil-water equations (Tanji, Wagenet, Selim and Iskandar). Those soils which exhibit swelling, or allow water to move rapidly through preferential channels, are difficult to treat analytically; for the same reasons, water movement through these soils is not well described by existing physically-based models. Solute movement in soils with well-defined, structured soils must be treated differently from homogenous soils. Models for these types of soils based on the soil-water equations have been used by Passioura, Wieringa and coworkers, but their solutions to these equations are complex. The problem also can be approached using a model (Addiscott) which divides the soil solution into mobile and non-mobile phases, using data from either the soil-water characteristic or aggregate size distribution. Solute movement between the phases can be expressed simply as equalization of concentrations, or more exactly as a diffusion controlled process. Such a model illustrates the broad principles of solute movement in structured soils, but is not mechanistic. It uses very simple inputs and is suitable for magenement purposes.

The hydrodynamic dispersion coefficient in the solute transport equation has been shown to be a function of soil-water content and pore-water velocity. It also has been shown to be non-normal in terms of spatial sample frequency distribution. Inclusion of the dispersion coefficient should be made in the solute transport equations. However, prior to this, the solution to the solute transport equation should be evaluated to ensure that numerical dispersion is absent. Numerical dispersion is an inherent error in certain finite difference solutions of the solute transport equation.

Classical ion-exchange equations, whose validity has been tested, should be used to describe ion exchange during solute transport in soils. Ion exchange involving equal-charged cations can be described by Vanselow-type equations, using equivalent fractions (or concentrations) in the adsorbed phase. Ion exchange involving cationic species with differently charged numbers (e.g. Ca^{2+}/Na^{+}) can be described by Gapon-type or Vanselow-type equations. Anion exclusion should also be considered; the extent of exclusion can be estimated on the basis of clay content, cation exchange capacity, etc. If appropriate ion exchange equations are unavailable, simple adsorption models (for example, linear adsorption isotherms) may be used to describe the retarded movement of ions. Ionic composition of the solution used to measure sorption isotherms should be similar to that encountered in irrigation water or soil solution.

Models to estimate soil pH or chemical processes influencing it are not well enough established at this time to be used in nitrogen models. Because of soil buffering, this is not an environmental property which would exhibit on a macroscopic scale wide swings during a growing season; thus, it can be considered a second order process for the present time.

Use of nitrogen models in salt affected soils or when salty waters are applied should recognize osmotic effects on microbial processes. Description is necessary of all solute concentrations so that a *total*, and not just nitrogenous, solute presence is predicted for such cases.

Because of the spatial variability associated with rate process parameters, a management level model using capacity coefficients may be an alternative approach (Rao, Davidson, Jessup). This type of model would provide less detail regarding water and solute fluxes, but would provide reasonable estimates of the position and distribution of soluble nitrogen species in the soil profile. Also the input parameters would provide reasonably good precision without extensive sampling. Although not a sophisticated model, it may be qualitative enough for many management-type decisions. These capacity-type models may in fact represent water and solute fluxes as accurately as the very mechanistic models which are limited by spatial variability of input parameters.

HEAT TRANSFER

Well defined, physically based mathematical models currently exist for describing diurnal temperatures in the soil profile. These models have been verified through laboratory experiments. Thus, accepted research-level models for predicting soil temperatures of selected soil depths are available for inclusion in nitrogen models. These models would provide temperature input information for biological processes. However, use of the models is limited by the fact that soil surface boundary conditions are generally not well defined and the heat transfer equations cannot be solved. Therefore, inclusion of current state-of-the-art heat transfer models may not be justified for inclusion in nitrogen models at the present time.

In view of the importance of describing soil temperatures for use in solving biological nitrogen submodels, it is suggested that an empirical approach be used for the present. This procedure would be based on annual temperature profile information. From this, daily changes in soil temperature could be made. This, however, would not be completely satisfactory in many cases for the top 15 cm of the soil.

GAS DISFFUSION IN RELATION TO DENITRIFICATION

The theory of diffusion in porous media is well understood, and many studies from the early 20th century onward have led to equations which closely describe experimental observations. Diffusion is the dominant process governing oxygen transport into the soil and N_2O and N_2 out, though mass flow may have some effect. Extreme limits for diffusion coefficients are well known from earlier studies.

The major problem in modelling the occurrence of anaerobiosis, and therefore the occurrence of denitrification, is that of defining the physical environment, its geometry, its dimensions, spatial variability, and three-phase composition in micro-environments.

Earlier models of diffusion considered the soil as a homogeneous, porous medium, and thus they were one-dimensional, with concentration gradients in the vertical direction only. The models for aggregated soils attempt to involve radial diffusion into aggregates of different sizes as well as diffusion down the profile. It is agreed that this is a better recognition of physical reality irrespective of whether spherical or other geometric shapes are postulated. Aggregate size distributions are easily measured and constitute some of the best independent data available for the model.

In sandy, structureless soils which are well aerated at depth, but where anaerobic conditions can occur in the biologically active uppermost layers the simple one-dimensional model concept is also inadequate. A possible approach here is to consider a layer through which some larger air-filled pores run but which, because of the random distribution of these pores, contain some zones sufficiently remote from them to allow anaerobic conditions to develop.

Spatial variability of diffusion coefficients has not been adequately investigated, but it is almost certain they are non-normal. This factor is as important as soil atmosphere gas concentrations of N_2O and N_2 in calculating fluxes from Fick's Law, and more data are urgently required.

N_2O in the gas phase is readily measured and N_2 evolved from added fertilizer N can be identified by ^{15}N labeling and mass spectrometry. However, the latter method does not measure N_2 from soil-derived sources.

Modelling of denitrification is at the research or conceptual level only, and is not appropriate for management purposes at our present state of knowledge.

VOLATILIZATION OF NH_3

Significant losses of nitrogen from the soil can occur through volatilization of NH_3. These losses occur when high concentrations of urea are placed on the soil surface. The volatilization occurs from shallow soil surface layers (0-5 cm) while very little NH_3 volatilizes from deeper soil layers. The diffusion of NH_3 through the soil can be modelled using Fick's diffusion equation. The major problem centers around estimating the diffusion coefficient as a function of soil-water content and soil type; however, some information is available from the literature. Volatilization of NH_3 from the top soil layers into the atmosphere can be modelled using the diffusion equation. This flux is a function of the boundary layer resistance which is controlled by wind speed and air stability. Information about this for laboratory conditions is available in the literature.

NH_3 volatilization from the soil may not, however, be a loss from the system since NH_3 can be adsorbed by the plant canopy. Scientific models for describing volatilization of NH_3 have been developed (Parton 1979, Van Veen 1978); however, these models are not appropriate for field applications.

AMMONIUM FIXATION

Soils that have potential for ammonium fixation are rare, but if high charge 2:1 clay minerals not saturated with K or NH_4 are present, they must be included in any model at the research level. In other cases, a suitable parameter in the ion exchange part of the model will handle ammonium which is temporarily, but strongly, held.

3.2 Soil microbiology

E. Bosatta, I.K. Iskandar, N.G. Juma, G. Kruh, J.O. Reuss, K.K. Tanji, J.A. van Veen

Micro-organisms in soils play a major role in the soil N-cycle, transforming N compounds into available and unavailable forms, mobile and immobile forms, oxidized and reduced forms, and gaseous and solute forms. The N transformations of interest to this workshop were nitrification, denitrification, mineralization-immobilization, and biological N_2-fixation.

Each of the above microbially-mediated reactions are examined relative to modelling approaches, appraisal of mathematical modelling and validation and to the effect of environmental and soil factors.

BIOLOGICAL N_2-FIXATION

Modelling of biological N_2-fixation in ecosystems is comparatively rare, in spite of the fact that in most natural terrestrial ecosystems this process is the principal external N-source. The process is usually included in models by a small assumed rate and the fate of this fixed N_2 is usually not clearly modelled as to its availability to plants.

Future modelling effort on N transformations in soil should be directed much more towards biological N-fixation than is done so far, especially in view of its increasing importance as an external N-source for agro-ecosystems.

NITRIFICATION

Nitrification is usually modelled as the result of the activity of chemo-autotrophic micro-organisms:
Nitrosomonas for oxidation of NH_4^+ and *Nitrobacter* for oxidation of NO_2^-. Heterotrophic nitrification is not explicitly considered in modelling.

Because only a few species of micro-organisms are involved the effect of the principal environmental factors affecting nitrification, temperature, pH, moisture and oxygen status is well defined and is over a much narrower range as compared to other processes, where a more diverse population of micro-organisms is involved. Thus, modelling of the effect of a particular environmental factor is comparatively easy and excellent fits with reality have been obtained. However, the combined effect of several factors has not yet been well defined. The lack of data and adequate mathematical expressions of the combined effects has appeared to be a very serious limitation to modelling, not only of nitrification, but also of the other N-cycle processes.

Another aspect which does not have had sufficient attention in modelling till now is the impact of microsites on nitrification. Since nitrification and denitrification do not occur simultaneously at a given microsite, the surface area of soil colloids and its micro-environment are of prime significance.

The mathematical modelling approaches to nitrification are the Monod (Michaelis-Menten) kinetics, chemical kinetics, and empirical equations. The application of Monod kinetics to soil nitrification was initially proposed by McLaren (1969). The more comprehensive Monod kinetic model (Van Veen, Frissel, McGill et al.) invokes the following

$$-d(S)/dt = 1/Y.dG/dt \qquad (1)$$

where S is the substrate (NH_4^+ or NO_2^-) concentration, t is time, G is biomass, and Y is the yield coefficient. Increase in growth is described by

$$dG/dt = \mu G \qquad (2)$$

where μ, the specific growth rate, is obtained from

$$\mu = \mu_m.(S)/(K_s + (S)) \qquad (3)$$

where μ_m is the maximum specific growth rate and K_s is the half-saturation constant. In most of the existing models limiting environmental factors are introduced by decreasing μ by several methods: multiplicative reduction factors, Liebig's Law of the Minimum Factors, and others such as the Arrhenius equation. However, it is well known that also the yield coefficient and the saturation constant are affected by temperature and pH.

Equation (4) can be obtained by combining equations (1), (2), and (3).

$$-d(S)/dt = \mu_m.G.(S)/Y.(K_s + (S)) \qquad (4)$$

Another approach, which can be derived from equation (4), assumes zero-order or first-order chemical kinetic models:

$$-d(S)/dt = K_0 \qquad (5)$$

$$-d(S)/dt = K_1(S) \qquad (6)$$

where K_0 and K_1 are respectively the zero- and first-order reaction rate constants. The decision on using whether zero- or first-order rate kinetics should, if possible, be based on a comparison of the actual N-concentration and the saturation constant. For nitrification a wide range of values of the saturation constant have been reported from < 1 to > 50 $\mu g.g^{-1}$ N with an average value of approximately 10 $\mu g.g$ N. In some instances, the two-step nitrification is modelled as one step, i.e., oxidation of NH_4^+ to NO_3^-.

Empirical rate equations have often been used when cause and effect relations are not known or when there is an advantage in fitting a model to site-specific experimental data. Some empirical models such as those advanced by Kruh and Segall have utility as they have been widely tested. However, empirical models do not have universal applicability as kinetic models do. In the mechanistic models the rate constants such as K_1 in equation (6) have values over a restricted range. The rate of reaction, -d(S)/dt, however, may vary widely because of (S) or the environmental reduction factors. The Monod (Michaelis-Menten) kinetic models are theoretically sound and more complete since they are linked to microbial biomass and enzyme-substrate kinetics. Such models have the capability to describe the entire time course of change including the lag time. Biomass-based models, however, require several parameters that are not commonly measured in soil N studies in the field and it is difficult to measure and/or validate microbial biomass. On the other hand, chemical kinetic models require minimal input data and are suitable for low substrate concentrations, but generally do not fit the entire time course of change. Another limitation to chemical kinetic models is that they assume unlimited biological potential, i.e., there are no upper or lower limits of control on the rate of reaction like the parameter μ_m in equation (3).

DENITRIFICATION

Since a diverse population of aerobic micro-organisms mediate NO_3^- reduction under certain O_2-limited conditions and in the presence of a wide variety of biodegradable organic carbon as an energy source, denitrification is less defined than nitrification. This is reflected in the present state of the mathematical models of denitrification.

Mathematical modelling approaches are similar to those for nitrification, including biomass-based kinetics, chemical kinetics, and empirical equations. But, unlike nitrification the physical environment also has to be modelled to establish when and where anoxic conditions prevail, including the occurrence of microsites (Smith, Van Veen and Frissel), Kruh and Segall). This physical modelling effort is discussed in section (3.1.) Also the effects of environmental factors are less defined as compared to nitrification because of the diverse population of denitrifying organisms. Under optimum conditions, denitrification proceeds rapidly until the substrate and/or one or more environmental parameters become rate-limiting. Mathematical simulation of the combination of environmental factors is limited in the same way as for nitrification.

The Monod kinetic approach may consist of single or double Michaelis-Menten kinetic modelling; as shown in equations 8 (Van Veen and Frissel) and 9, respectively.

$$d(NO_3)/dt = K_d.(NO_3)/(K_{NO_3} + (NO_3)) \tag{8}$$

$$d(NO_3)/dt = K_c.(NO_3)/(K_{NO_3} + (NO_3)).(\text{soluble Org.C})/(K_{Sol.C} + (\text{Soluble Org. C})) \qquad (9)$$

where K_d and K_c respectively are the maximum denitrification rate, and K_{NO_3} and $K_{Sol.C}$ respectively are the half-saturation constant. Equations (8) and (9) may be extended to include biomass population and the specific growth rate.

Because it is difficult to ascertain the Michaelis-Menten constants and the denitrifiers, chemical kinetics are used by other modellers (Mehran and Tanji, Tanji et al., Rao et al., Selim and Iskandar, Wagenet, Krug and Segall). However, it is disputable whether to use first- or zero-order kinetics with respect to NO_3^-, on the basis of the value of the saturation constant, K_{NO_3}, of which values have been reported from 0.09 $\mu g.g^{-1}$ N (for liquid cultures) up to 40 $\mu g.g^{-1}$ N (in soil). Some modellers explicitly allow denitrification to occur only, when they assume, that anaerobic conditions exist e.g. when the pressure head is 15 cm or less or when soil water content is 80% or greater than saturated water content (Selim and Iskandar).

The Michaelis-Menten and chemical kinetic approaches of modelling have the potential of simulating denitrification better than chemical kinetics if they consider soluble organic carbon in addition to NO_3^-. The former, however, assumes the rate of denitrification to be bounded by the upper and lower biological limits, while the latter does not. Van Veen and Frissel simulated the production of soluble organic C in their mineralization-immobilization modelling and then assumed zero-order kinetics with respect to NO_3^-. Experimental validation of models for denitrification is hampered by difficulties in direct measurements of the denitrification products as well as identification and counting of denitrifiers. Denitrification cannot be accurately predicted without an estimate of substrate availability, preferably soluble C. This implies coupling of the N cycle with the C cycle. Unfortunately, soluble C estimation is probably one of the most difficult aspects of C modelling.

HYDROLYSIS OF UREA

The hydrolysis of urea is a well documented enzymatic process. It is dependent mainly on soil pH, urea concentration and soil temperature. In most cases, the ability of the soil to buffer against pH change will make unnecessary the description of dynamic soil pH status as a mediator in hydrolysis. Urine patches and similar localized, highly concentrated organic concentrations represent special cases where this assumption may not be valid. Michaelis-Menten kinetics are a reasonable and acceptable means of characterizing hydrolysis as a function of urea concentration. Description of temperature fluctuations in the surface soil needs to be provided in detailed models. This probably does not need to be included in management-level models as the hydrolysis of urea is usually fairly rapid, and description of the process as a function of temperature might therefore be of a second-order resolution.

MINERALIZATION-IMMOBILIZATION

The process of mineralization and immobilization are greatly determined by the large diversity of the micro-organisms involved. This is also reflected in the effects of environmental factors. The processes occur over a very wide range of temperature, pH and moisture content, and under both aerobic and anaerobic conditions.

Another determining factor is the strong relationship between the soil C- and N-cycle. The modelling apporaches can be divided into three categories:

1. Models which do not consider C decomposition and predict mineralization of N using first-order kinetics (e.g. Tanji et al. or use a pseudo Arrhenius equation (Addiscott).
2. Models which consider C and N and use the C/N ratio of substrates as the parameter determining whether net mineralization or net immobilization occurs.
3. Models which consider C and N as substrates for the biomass.

In these models, the net mineralization or immobilization is the result from the balance of gross mineralization and gross immobilization rates. As these processes involve microbial growth and decay, several approaches have been used in describing microbial activity:

a. The biomass is divided into two components: bacteria and fungi. These components have different C/N ratios, which can vary within certain limits (McGill et al.).

b. The biomass has a fixed C/N ratio and the total biomass is involved in the decomposition of each of the different organic C-substrates (Bosatta).

c. The biomass is assumed to have a fixed C/N ratio and a fraction of the biomass is involved in the decomposition of each of the different organic C-substrates (Van Veen and Frissel).

d. The biomass is assumed to have a fixed C/N ratio and has unlimited biological potential to decompose C-substrates under most conditions. Thus, it is the C-substrate concentration rather than the size of biomass that is used to calculate the amount of C decomposed (Juma and Paul).

In the comprehensive models which include biomass it is highly desirable to include explicitly biomass turnover. Considering the fact that most of the organic material entering the soil such as roots and litter as well as native soil organic matter is taken up and transformed, albeit with very different rates, by the biomass, the dynamics of soil organic matter are primarily determined by the growth and death of micro-organisms. However, the present knowledge on the quantity and the quality of organic materials being released during biomass turnover is very limited and for the greater part derived from laboratory or wastewater experiments.

In most of the comprehensive models, the exogenous and soil substrates are divided into several components. This approach attempts to divide the carbon substrates according to their relative availability to the biomass. Although this approach is very superior to a description in which soil organic matter is considered to be an entity, it should be pointed out that the possibilities to measure quantity and turnover rate of the several soil organic matter fractions are limited. The decomposition of these substrates are described by Monod (hyperbolic) kinetics and first order kinetics.

The advantages and disadvantages of these descriptions are:

Monod model

In this model the values of μ_m and K_s are needed. The μ_m and K_s values for various substrates have been determined for wastewater treatments but with a few exceptions not for soil. It sounds reasonable to assume that the maximum specific growth rate is of the same order of magnitude for both the wastewater and soil system, because it refers to the intracellular systems. However, the saturation constant as used in the soil organic matter models is a combination of two constants: (i) the affinity constants for the substrate and (ii) a constant which accounts for spatial availability of the substrate. The latter does not allow for a determination of K_s other than in the soil system itself.

First-order kinetic model

In these models the decomposition of C is limited by the substrate concentration and not by the biological potential of the biomass. It is readily applicable to the soil system as decay rate constants are available (Paul and Van Veen, 1978).
As mentioned before, there is no upper or lower limit to the decomposition rate, which is in contradictory to experimental results.

CONCLUDING REMARKS

Modelling efforts on soil N transformations vary widely in their complexity and resolution. Although the more simple chemical kinetic and some empirical approaches have their uses, they usually do not apply over widely ranging conditions and/or time because there is no explicit treatment of microbial activities. Therefore, the more comprehensive Monod kinetic models have more biological significance and generality. Since microbes are central to the dynamics of soil N, it is highly desirable to describe explicitly the activity, growth, and death of the microbes in N transformations. In these comprehensive models it is necessary to model not only the N-but also the C-cycle, since the latter is usually the rate limiting nutrient. This requires fractionation of soil organic matter as the substrate for micro-organisms. Modern techniques of measuring the growth and activity of the biomass as well as use of tracer techniques would provide further understanding and a better data base for simulation modelling.

The degree to which environmental factors such as temperature, soil moisture, pH, etc. affect microbial N transformations is strongly dependent upon the diversity of the involved microbial population. If only a few genera are involved, as in nitrification, they are much more sensitive to the environmental factors, in contrast to the total microbial population participating in immobilization. Hence, the more significant environmental and soil factors should be considered in modelling soil N transformations. Data on the effect of a single environmental factor are superfluous but data on the combined effects are hardly available. This makes equations which take care of combined effect in simulation models rather arbitrary. This is considered to be one of the most serious limits to the present models.

It is clear that the behaviour of soil N as affected by microbially-mediated reactions is very significant and complex. It is also clear that mathematical and computer capabilities are available but that the present knowledge on the various aspects is far from complete.

3.3 Soil-plant relations

H. Breteler, D.J. Greenwood, I. Petterson, J.S. Russell, D. Sauerbeck, F. van Dorp,
H. van Keulen, H.G. van der Meer

ANALYSIS

The group considered the various plant processes in the models presented at the workshop. A classification of the main plant processes in the several models was made. This classification is incorporated into Table 1. Each of the approaches used for the different processes was examined and compared for the different models. This was used as a basis for identifying the limitations of existing knowledge and for pinpointing areas of greatest need.

ROOT GROWTH

Most of the existing models rely on some empirical relations and it is believed that there is a considerable need for more mechanistic models for root growth. There is a special need to devise means of taking account of the balance between root and shoot growth and the effects of soil physical conditions on root distribution in the soil. Attention should also be given to distinguishing between root weight or root volume and root length. In our view the lack of validated root growth models is a major limitation to the development of crop-soil models.

WATER UPTAKE

The treatment of water uptake has been based to a large extent on well established principles about the movement of water through soil and plants. When the actual transpiration rate is similar to the potential tmaspiration rate, almost all models, considering water uptake, are based on Darcy type equations relating water flux to gradients in water potential of the entire soil plant system. They rely on the root distribution and give good predictions of the distribution of water beneath the crop. However, when the crop is under stress and water uptake is less than the maximum, the models are rather more empirical and thus may be of less widespread applicability.

We foresee there is a need to develop models which incorporate water potential within the plant as a key feature. We also believe that there is a need to develop relationships between water potential in the plant and photosynthesis, growth and the distribution of assimilate.

NITROGEN UPTAKE

The treatment of the uptake of nitrogen by plant roots is far less based on fundamental concepts than that of water. Nevertheless the main factors that are known to affect nitrogen uptake are incorporated in one model or another. These are (1) the dependence of the uptake of nitrate on the presence of ammonium, (2) the effect of concentration at the root surfaces on the rate of uptake and (3) the dependence of uptake on the demand of the crop for nitrogen and the extent and distribution of the root system.

Much available knowledge, however, does not appear to have been fully utilized in the development of the models. Especially important are:

1. A great deal of information exists about the effect of NH_4^+ or NO_3^- concentration on the uptake rate of the two ions. In particular the rate of NO_3^- uptake by plant roots is unaffected by nitrate concentration over a wide range provided this exceeds a very low value of about 0.1 mM. It seems reasonable to consider nitrate uptake as governed by an ON/OFF switch depending on the concentration at the root surface.
2. The absorption of NO_3^- increases pH and absorption of NH_4^+ decreases pH in ways that can be readily calculated. The effects are very large and we believe that they could have considerable influence on root and microbial activity of the rhizosphere, particularly in poorly buffered systems.

The group identified that progress could be much improved if there were better conceptual sub-models for the following processes:

- The dependence of nitrogen uptake by crop roots on the N status and the physiological condition of the plant.
- The transport of nitrate through the soil and especially the way this is affected by soil water content and properties of the root-soil interface.
- The proportion of roots that must take up nitrogen to satisfy the needs of the whole crop.

ROOT DEBRIS AND EXUDATION

Most models for roots take no account of the well established fact that a substantial proportion of the roots is subsequently metabolized by soil organisms. A considerable proportion of the roots appears as inanimate material in the soil and as constitutents of micro-organisms. We believe that it is important to incorporate some concepts representing these processes into whole plant-soil models. There are two reasons for this view. (1) Unless account is taken of the process, present concepts of partition of assimilate between root and shoot will grossly overestimate the amount of active root which, in turn, will have indirect effects on predictions of water and N uptake. (2) Breakdown of the roots greatly influences the size of the biologically active pool of organic matter in rhizosphere and soil and can thus have a considerable influence on processes such as denitrification. Indeed we believe that this process could explain the difference between the nitrogen economy of cropped and uncropped soils.

We recognize that to develop these concepts there is a need for further quantitative experimental data.

DRY MATTER PRODUCTION

Several models have related total dry matter production to the transpiration rate or the ratio of actual to potential transpiration. The choice depends on the environmental conditions, but with this limitation the models appear to give a good description of the experimental data when yields are not limited by nutrients in general.

Nevertheless there are a number of ways in which substantial improvements could be made. These include the development of better quantitative theories for:

1. The influence of crop nitrogen status on photosynthesis, growth rate and the partition of assimilate between different pools of the plant.
2. The interaction between N and water status on dry matter production and water use.

CONCLUSIONS

The general conclusion is that the understanding of water transport in soils and plants is much greater than our understanding of root development, root function and nitrogen nutrition. It is recognized that major limitations to progress are the lack of technology for studying roots in the soil and the problems of validating complex models.

3.4 Model validation

M.J. Frissel

It was unanimously concluded that techniques for the validation of the models are insufficient. Some particular problems which were discussed are:

1. Correctness of computer program, i.e. does the program really describe the concept? Programming errors such as the use of a + sign instead of a - sign or the omission of a correction factor which is close to 1 are difficult to eliminate. In case two modellers use exactly identical concepts it is possible to use each others data sets. Errors may be detected in that case. However, a planned inter-model comparison failed because there exist always small differences in concepts invoking different equations thus requiring different data sets.

The preparation of a standard data set which covers these differences in concept (i.e. contains optional parameters) and thus can be used by many modellers was highly recommended. A few participants are working along this line.

2. Programs may be checked by simplifying the program so far that analytical solutions can be applied. Most nitrogen programs are, however, so complex that this technique can hardly be used.

Another check is the introduction of a summation procedure in the program of all N present in the separate pools. The total amount of N should be constant with time. An increase of a decrease indicates an error. Because, however, accumulated losses and gains, e.g. from atmospheric nitrogen, also have to be included, this technique is not popular.

3. Experimental data which can be used for model validation are scarce. Model developers are faced with the situation that their equations contain more unknown parameters than the number of independent data sets which are available. From a mathematical point of view data sets of different years or plots, from the same experimenter, are often similar so that they do not much contribute to the assessment of the parameters. On the other hand, extreme conditions, which may be a flood for the one and a drought for the other, provide a much better assessment of certain parameters. The only problem is that under such extreme conditions the conceptual model, which was developed for non-extreme conditions, may no longer be valid.

The aforementioned problems make a validation of models on N behaviour in soil difficult and questionalbe. It must, however, be stressed that the first objective of the majority of the models is not prediction, but rather to obtain a better understanding of the terrestrial N-cycle. The model is a tool in studying the complex interactions between all processes which control the N behaviour in soil. Only when this state is passed and understanding is sufficient predictive models could be developed.

4. Description of models

4.0 Format of descriptions

With a few exceptions all models are described according to the same format. Descriptions are separated into the following parts.

1. Name of model or program
2. Systems modelled
3. Objective
4. Time scale
5. Diagrams
6. Pools (levels)
7. Governing equations
8. Input parameters
9. Output, verifiable variables
10. Observations
11. Comparison results
12. Limits and limitations
13. Computer
14. Program language
15. Running time/cost
16. Users
17. Developer and principal contacts

4.1 Water and nitrogen fluxes in the root zone of irrigated maize

K.K. Tanji, M. Mehran and S.K. Gupta

1. NAME OF MODEL OR PROGRAM

UCD-RANN MODEL

2. SYSTEMS MODELLED

Corn field - irrigated and fertilized, one-dimensional transient flow, Mediterranean climate.

3. MODELLING OBJECTIVES

a. Simulate the physical, biological and chemical processes and conditions in the root zone of corn fields.

b. Develop capability to simulate water and nitrogen fluxes over small time and space increments for a growing season.

c. Verify the water and nitrogen submodels with data from the corn field trials at Davis, California.

d. Utilize the models to interpret and evaluate experimental results such as spatial variability of soil hydraulic conductivity.

e. Apply the model to other soil-plant-water systems where sufficient input data and validation data are available.

4. TIME SCALE

This is a transient model designed to simulate changes in fractions of an hour to some maximum time span desired by the modeller, provided the time variation of boundary conditions can be handled by computer storage.

5. DIAGRAM

Figure 1. Simplified block diagram of the water and N transport submodels.

Figure 2. Mechanisms and processes modelled in soil N simulation.

6. POOLS (LEVELS)

Not applicable.

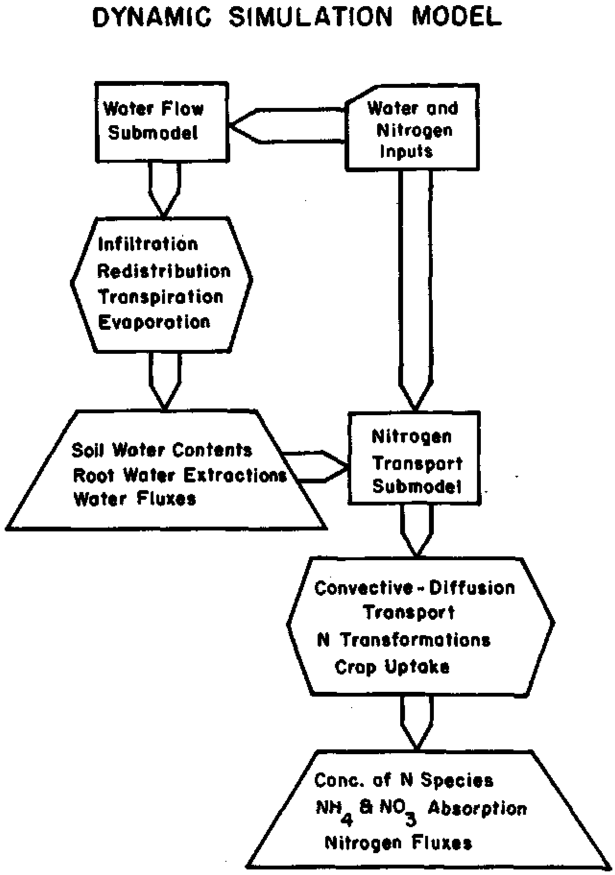


Fig. 1. A simplified block diagram of the water flow and N transport submodels.

7. GOVERNING EQUATIONS

a. *One-dimensional nonsteady flow of water (Gupta et al., 1978)*

$$C(\theta)\,\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(h)\,\frac{\partial H}{\partial z}\right] - S \qquad (1)$$

where

$C(\theta)$ = differential soil water capacity, $\frac{d\theta}{dh}$, $cm^3\ cm^{-3}\ cm^{-1}$
θ = volumetric water content, $cm^3\ cm^{-3}$
h = pressure head, cm
$K(h)$ = hydraulic conductivity, $cm\ d^{-1}$
H = total head, $h + z$, cm

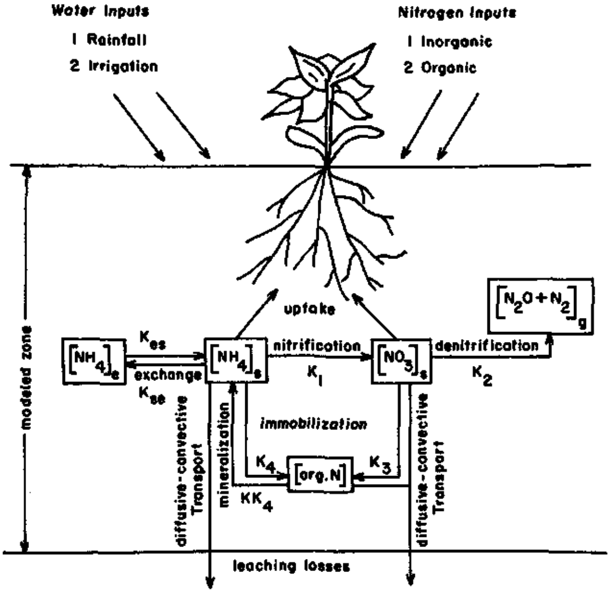


Fig. 2. Mechanisms and processes modelled in the N transport submodel.

S = sink term for root extraction, $cm^3\ cm^{-3}\ d^{-1}$
t = time, d
z = soil depth, cm.

Equation (1) is subject to the usual initial and boundary conditions including semi-infinite soil depth (Gupta et al., 1978), and solved by an implicit finite difference approximation method.

To compute θ and water-flux (q) for each node, functional relations between θ and h and also between K and h were developed. The measured field data on θ and h was related by

$$\theta = b_0 + b_1 \log h + b_2 (\log h)^2 \qquad (2)$$

Then a separate program was used to estimate K from h extrapolating from the wet to the dry range using the Millington and Quirk method (1961) along with the Jackson et al. matching factor (1965). K and h was related by

$$\log K = a_0 + a_1 \log h + a_2 (\log h)^2 \qquad (3)$$

The sink term S for root water extraction in equation (1) was defined by the Nimah and Hanks' (1973) macroscopic model

$$S = K(h) \left[\frac{h_r - h}{R(z)}\right] - \frac{RDF(z)}{\Delta z \Delta x} \qquad (4)$$

where

h_r = derived root water pressure at the root-soil interface, cm
R = radius of water flow to roots, cm
RDF = root distribution function defined as the proportion of roots in Δz
Δz = radial distance between roots, cm
Δz = soil depth, cm.

RDF is related to the root length density by

$$RDF(z) = \frac{L_{v(z)}}{\Sigma L_v} \qquad (5)$$

where

$L_{v(z)}$ = root length density in z soil depth, cm cm^{-3}
ΣL_v = total root length density in the root zone, cm cm^{-3}

$$L_{v(z)} = 3.5\ [1 - 1.0 \exp\ (-0.02t)] \qquad (6)$$

for corn grown in the Yolo soil (Acevedo, 1975).

Radial distance between roots is computed from

$$x = \left[\frac{1}{\pi L_v}\right]^{\frac{1}{2}} \qquad (7)$$

Since Nimag and Hanks (1973) inputs RDF and assumes Δx to be unity, this model is an extension of the former. Extraction is allowed to proceed between the prescribed limits of saturation and wilting point, assumed to be 10 bars, as well as the imposed potential evapotranspiration.

The potential transpiration (E_{pt}) when soil moisture is not limited is estimated from potential evapotranspiration (ET_p) and leaf area index (LAI) by the Ritchie and Burnett method (1971).

$$E_{pt} = ET_p\ (-0.21 + 0.7\ LAI^{\frac{1}{2}}) \qquad (8)$$

over the range of $0.1 \leq LAI \geq 2.7$ for corn. When LAI > 2.7, $ET_p = E_{pt}$ and when LAI < 1.0, E_{pt} is considered negligible.

The actual rate of transpiration is computed by assuming linear decrease (Thornthwaite and Mather, 1955)

$$T = E_{pt}\left[\frac{SWS}{AW}\right] \tag{9}$$

where

SWS = actual soil water stored at any given time in the root zone, cm
AW = so-called available water between wilting point and field capacity, cm.

The nonlinearity of equation (1) is treated by one of several iterative schemes (Gupta et al., 1978). In this model, mass balance is used as an additional criterion for iteration. At each time step, the total moisture content are compared between two independent means: (1) estimated from predicted values and (2) estimated by mass balance, i.e., initial condition at each time step + inflow - outflow - extraction - evaporation. If the absolute difference between these two are more than the prescribed limit (e.g., 0.1 cm), the iterations are carried out with new values of K and C for each node. If the solution does not converge within ten iterations, Δt is reduced in half and the whole process is repeated. This model is also being used to obtain further insight into the complexities of field soil water cycle (Biggar et al., 1977). One major application is the evaluation of spatial variability of soil hydraulic conductivity.

Simmons et al. (1979) analysed heterogeneity of hydraulic conductivity by

$$K = \alpha^2 K_m \exp[\beta(\theta - \theta_0)] \tag{10}$$

where

α = scale factor
K_m = scale mean hydraulic conductivity, cm d^{-1}
θ_0 = saturated water content, $cm^3\ cm^{-3}$
β = location-dependent parameter.

And saturated hydraulic conductivity, K_0, is defined by

$$K_0 = \alpha^2 K_m \tag{11}$$

b. *One-dimensional nitrogen flow (Tanji and Mehran, 1979)*

$$\frac{\partial(\theta c)}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z} + \frac{C\lambda(z,t)}{\theta} - \frac{\rho}{\theta}\frac{\partial E}{\partial t} + S_c \tag{12}$$

where

c = concentration of mobile N species, $\mu g\ cm^{-3}$
D = apparent diffusion coefficient, $cm^2\ d^{-1}$

v = pore water velocity, cm d^{-1}
ρ = soil bulk density, g cm^{-3}
E = concentration of N in the exchanger phase, $\mu g\ g^{-1}$
λ = root absorption coefficient, dimensionless
S_c = sources or sinks.

Equation (13) is subject to the usual initial and boundary conditions (Tanji and Mehran, 1979).

The term S_c includes all of the transformations (Figure 3) contributing to c as sources and/or sinks. Assuming that all transformations obey first-order kinetics (Mehran and Tanji, 1974) and that NH_4^+ and NO_3^- are the only mobile solute species, differential equations describing the rate of change of all N species under consideration are as follows:

$$(1 + R_f)\frac{\partial A}{\partial t} = D_A\frac{\partial^2 A}{\partial z^2} - v\frac{\partial A}{\partial z} + \frac{A\lambda(z,t)}{\theta} - [K_1(z) + K_4(z)]A + K_5(z)\frac{\rho}{\theta}F \tag{13}$$

$$\frac{\partial B}{\partial t} = D_B\frac{\partial^2 B}{\partial z^2} - v\frac{\partial B}{\partial z} + \frac{B\lambda(z,t)}{\theta} - [K_2(z) + K_3(z)]B + K_1(z)A \tag{14}$$

$$\frac{\partial E}{\partial T} = K_{ex}\frac{\partial A}{\partial t} \tag{15}$$

$$\frac{\partial F}{\partial t} = K_3(z)\frac{\theta}{\rho}B + K_4(z)\frac{\theta}{\rho}A - K_5(z)F \tag{16}$$

$$\frac{\partial G}{\partial t} = K_2(z)\frac{\theta}{\rho}B \tag{17}$$

where

A = concentration of solution NH_4^+, μg N cm^{-3}
B = NO_3^- concentration, μg N cm^{-3}
E = concentration of exchangeable NH_4^+, μg N g^{-1}
F = organic N concentration, $\mu g\ g^{-1}$
G = gaseous N concentration, $\mu g\ g^{-1}$
K_{ex} = coefficient of exchange reaction, $cm^3\ g^{-1}$
D_A and D_B = apparent diffusion coefficient for NH_4^+ and NO_3^-, $cm^2\ d^{-1}$
R_f = $\rho K_{ex}/\theta$
K_1, K_2, K_3, K_4, K_5 = transformation rate constants for nitrification, denitrification, immobilization of NO_3^-, immobilization of NH_4^+, mineralization, respectively, d^{-1}.

Prediction of nitrogen leaching losses at any depth for all time levels requires simultaneous solution of the above differential equations. Equations (13) through (17) are solved numerically using an implicit finite difference scheme. To ensure the accuracy of this numeric scheme, a check on mass balance similar to the water flow submodel was carried out.

8. INPUT PARAMETERS

a. *Water flow submodel*

Number of nodes, depth segments, and material properties (layers with distinct hydraulic properties).

Crop data (dates of planting and harvest, read number of days roots take to grow to various depths).

Read factors to convert daily PET to hourly values.

Read irrigation and rainfall (amount, time, and date).

Parameters for hydraulic conductivity (initial values of θ and h, coefficients for equations (2) and (3), θ at steady state infiltration, saturated and dry K).

Moisture tension and water content limits (total initial θ, maximum depth of ponding, maximum and lowest limits of suction, saturation and dry θ).

Controlling factors for time steps and iteration (maximum time steps during irrigation and nonirrigation periods, minimum limit of time step if mass balance or iteration does not converge, maximum difference in mass balance).

Coefficients for spatial variability of K (α and β for equation (10)).

b. *Nitrogen flow submodel*

Requires output data from water flow submodel (θ, q, S).

Initial profile distribution of solution and exchangeable NH_4^+, NO_3^-, organic N, and gaseous N.

Number of nodes and depth increments.

Specification of initial time and space increments.

Root absorption coefficient for NH_4^+ and NO_3^-.

Apparent diffusion coefficient for NH_4^+ and NO_3^-.

Soil bulk density.

First-order transformation rate constants and ion exchange constant.

Applied concentrations of NH_4^+ and NO_3^- in irrigation water and rainfall.

Applied fertilizer N.

9. OUTPUT, VERIFIABLE VARIABLES

Water content, water-flux, water uptake.

Concentration of all N species in the soil profile.

Mass of NO_3^- and NH_4^+ taken up by corn.

Mass of NO_3^- and NH_4^+ leached past the root zone.

10. OBSERVATIONS

This modelling effort (Tanji and Mehran, 1979) was supported by the Research Applied to National Needs (RANN) Division of the National Science Foundation (NSF) as part of a larger research activity entitled Nitrate in Effluents from Irrigated Agriculture (Pratt, 1979). The experimental data base for this simulation modelling was derived from a corn monoculture field experiment conducted for five years at the Davis Campus of the University of California (Broadbent and Carlton, 1979; Biggar et al., 1979).

The irrigation regime consisted of 20-, 60-, and 100-cm of sprinkler irrigation during the growing season (May through September), which corresponded to 1/3, 3/3, and 5/3, respectively, of the average corn ET at Davis. All plots were pre-irrigated prior to seeding so that the surface 3 m of the soil contained 100 cm of water. Fertilizer was applied at 0-, 90-, 180-, and 360-kg N/ha of $(NH_4)_2SO_4$ at planting time in the 5 cm depth. The 12 field plots (6.1 m x 9.1 m) were replicated four times. Each of the plots were instrumented with soil solution suction cups as well as tensiometers. Water contents were

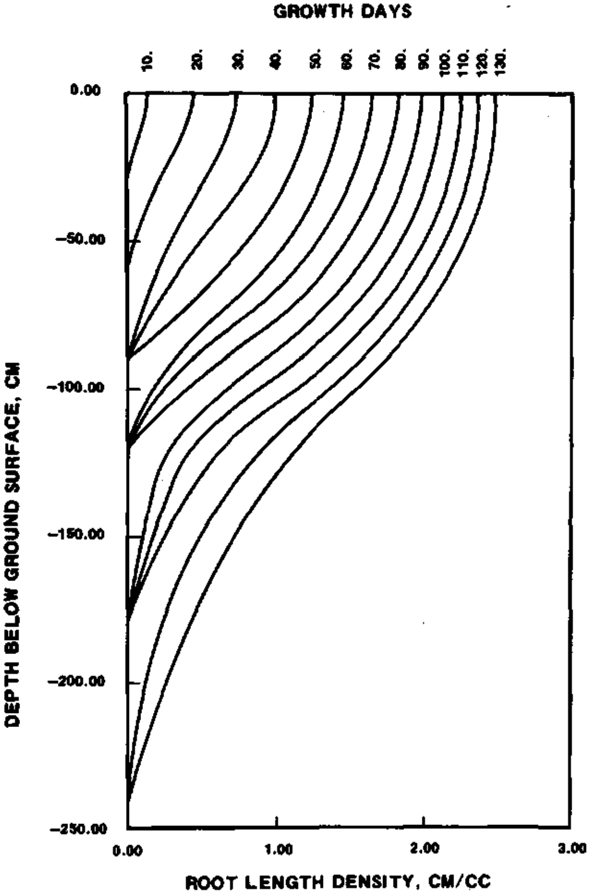


Fig. 3. Root length density for various growth days of maize.

measured by a neutron probe. The tops were harvested for grain and stalk measurements. The soil was sampled after each harvest.

11. COMPARISON RESULTS

The water flow submodel was used to simulate the 1/3, 3/3, and 5/3 ET treatments of the 1975 growing season, while the N flow submodel was used to simulate the 0-, 90-, 180-, and 360-kg N/ha treatments of the 5/3 ET irrigation regime of the 1975 growing season. In addition to verified results, simulated results are presented herein to give a more comprehensive description of model capabilities.

Figure 3 gives the simulated root length density based on equation (6).

Figure 4 shows the simulated profile θ for the 20-, 60-, and 100-cm treatments.

Figure 5 contains plots of seepage at the 20-cm depth along with depths of sprinkler irrigations biweekly.

Figure 6 presents the validation of simulated θ for the three irrigation treatments at selected days after planting. Note that simulated values are well within the standard deviations of measured data.

Table 1 summarizes simulated results evaluating the spatial variability of K. Scale factor of 0.404 is greater than the mode but less than the arithmetic average while 2.364 represents 10% of the higher saturated K.

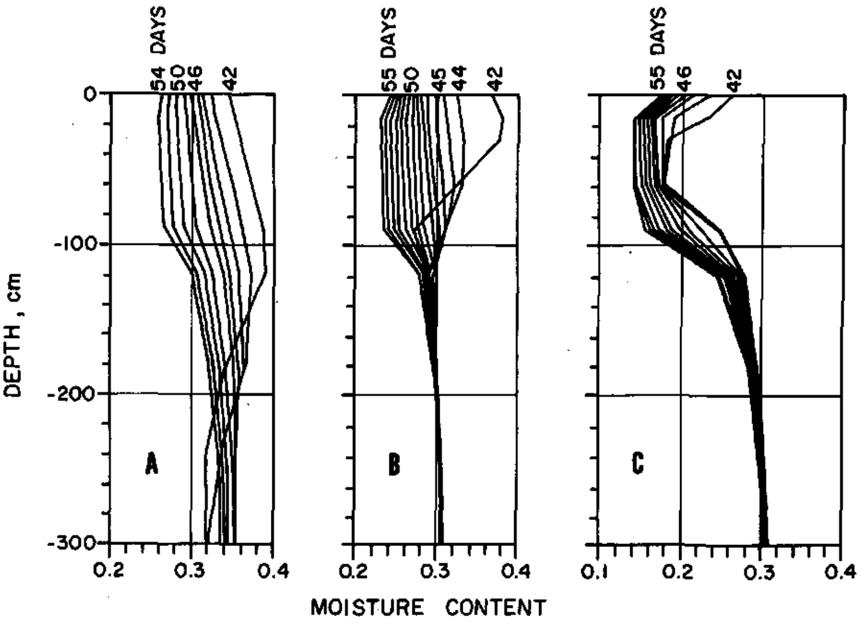


Fig. 4. Soil water content (cm^3 cm^{-3}) simulation for the third irrigation cycle in the three different treatments: A (5/3 ET), B (3/3 ET), and C (1/3 ET).

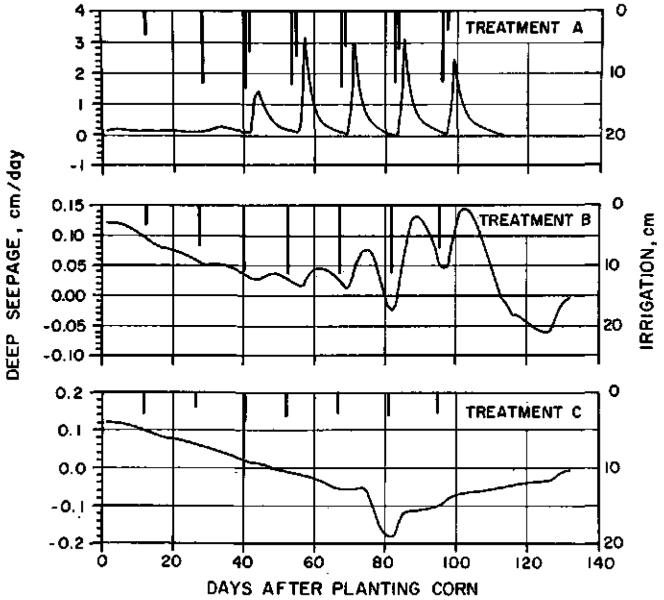


Fig. 5. Daily seepage (cm d^{-1}) at the 20-cm soil depth. Note: seepage downward is considered positive.

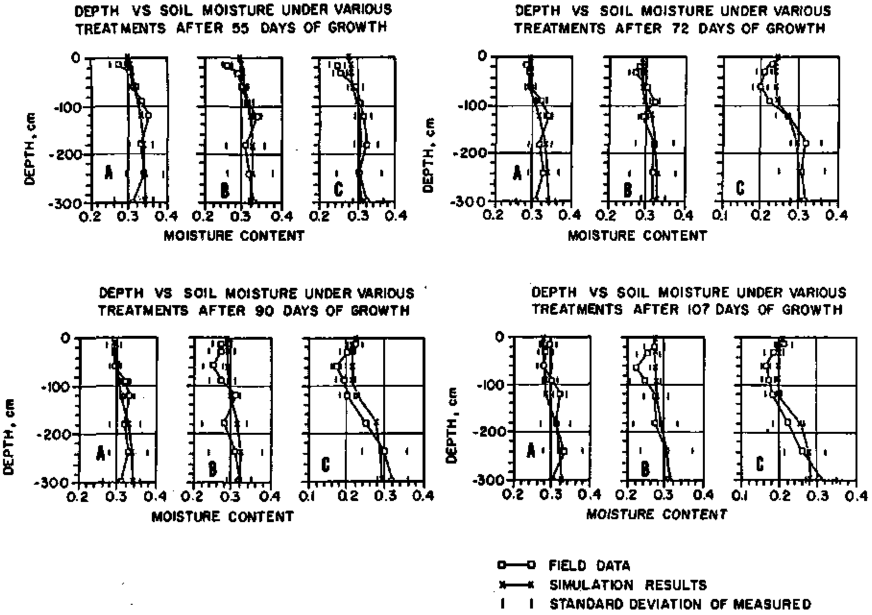


Fig. 6. Measured and predicted soil moisture over the maize growing season.

Table 1. Evaluation of spatial variability in soil hydraulic conductivity (equations (10) and (11)[1]).

	100-cm irrigation (5/3 ET)		20-cm irrigation (1/3 ET)	
Scale factor α	0.404	2.364	0.404	2.364
Saturated K, cm d^{-1}	2.0	63.3	2.0	63.3
Soil water after pre-irrigation, cm	105	105	105	105
Irrigation during cropping	101.9	101.9	20.1	20.1
Transpiration, cm	48.2	34.2	35.6	22.8
Evaporation, cm	6.4	6.4	6.7	6.7
Seepage, cm	76.8	118.7	22.6	56.3
Soil water after cropping, cm	70.2	42.3	60.2	39.3

Table 2. Sensitivity analysis for mineralization in the 0-kg ha^{-1} N treatment.

Case	Mineralization rate K_5	Nitrification rate K_1	Denitrification rate K_2	Uptake coefficient	Nitrogen uptake	Residual inorganic N	Leaching losses
	d^{-1}				kg ha^{-1} N		
	Calculated:						
1	10^{-4}	.4	.005	1.00	48	139	169
2	10^{-4}	.4	.005	1.25	57	134	159
3	0.5×10^{-4}	.4	.005	1.00	31	87	117
4	$K_5 = 10^{-4}$ in top 30 cm, $K_5 = 10^{-5}$ in 30-300 cm	.4	.005	1.25	51.5	105	108
5	10^{-4} only in the top 30 cm	.4	.005	1.00	43	62	76
6	10^{-4} only in the top 30 cm	.4	.005[2]	1.25	57	69	70
	Measured:						
					77	117	

Table 3. Comparison between measured and computed results for the 5/3 ET irrigation regime in kg ha^{-1} N.

Application rate	Plant uptake		Residual inorganic N		Calculated leaching losses
	Measured	Calculated	Measured	Calculated	
0	77	57	117	69	70
90	155	121	137	91	77
180	214	202	134	89	123
360	283	260	295	260	300

[1] $\beta = 13.0$, $K_m = 5.8$ cm d^{-1}, $\theta_o = 35$ cm^3 cm^{-3}.

[2] Only in the lower 150 cm of the soil profile.

Table 2 presents sensitivity analysis to ascertain the most likely value for mineralization rate constant. This parameter is of most importance in this soil because of the large source of organic N, about 22,000 kg ha^{-1} for a 3 m profile.

Table 3 summarizes the validation of computed uptake of N and residual inorganic N while Figures 7-10 contain comparisons of measured and simulated NO$_3^-$ in the soil for the 0-, 90-, 180-, and 360-kg ha^{-1} N rates, respectively, of the 5/3 ET treatment at eight selected days after planting.

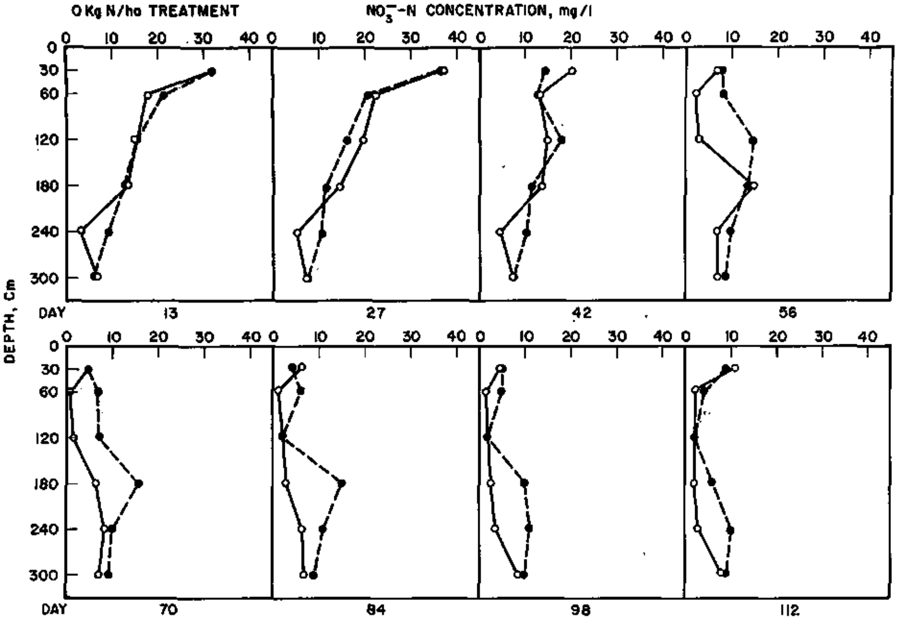


Fig. 7. Measured (solid line) and simulated (broken line) NO$_3^-$ concentration profiles at different days for the 0-kg ha^{-1} N treatment of the 5/3 ET irrigation regime in 1975.

12. LIMITS AND LIMITATIONS

Maximum time step during nonirrigation = $\leq$ 1.0 d.

Maximum time step during irrigation = $\leq$ 1.0 h.

Minimum limit of time step = half of existing Δt if mass balance or iteration does not converge.

Maximum difference in mass balance of water = 0.1 cm.

Space step for water flow = variable (30-60 cm), depending upon availability of input data.

Maximum time step for N submodel = $\leq$1.0 h.

Space step for N flow = 5 cm used but can be variable.

The limits in Δt and Δx have not been fully explored for stability of numeric scheme. The

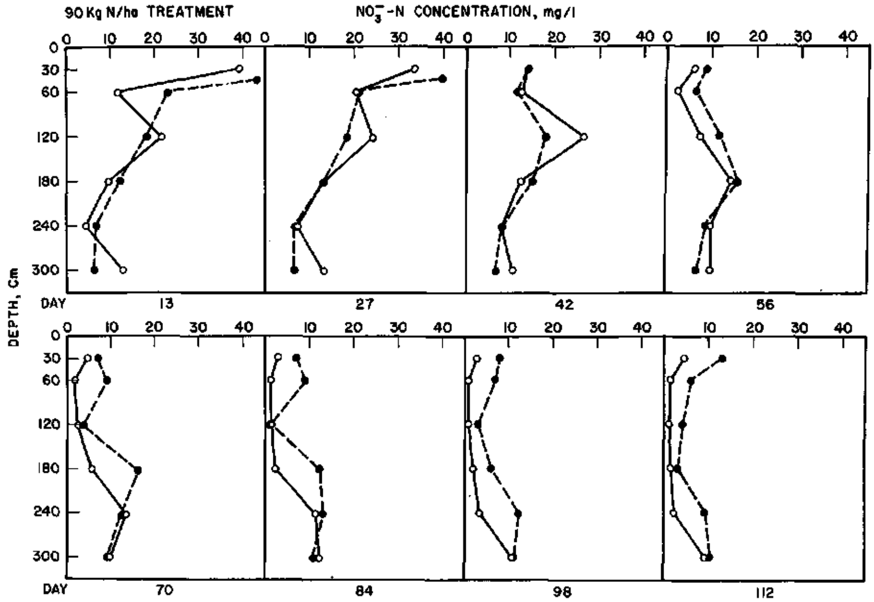


Fig. 8. Measured (solid line) and simulated (broken line) NO$_3^-$ concentration profiles at different days for the 90-kg ha^{-1} N treatment of the 5/3 ET irrigation regime in 1975.

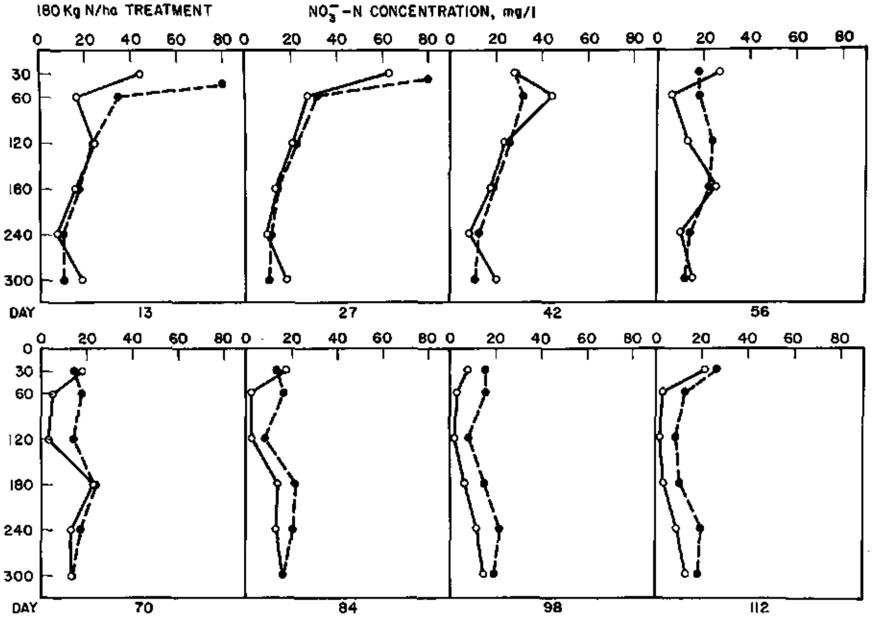


Fig. 9. Measured (solid line) and simulated (broken line) NO$_3^-$ concentration profiles at different days for the 180-kg ha^{-1} N treatment of the 5/3 ET irrigation regime in 1975.

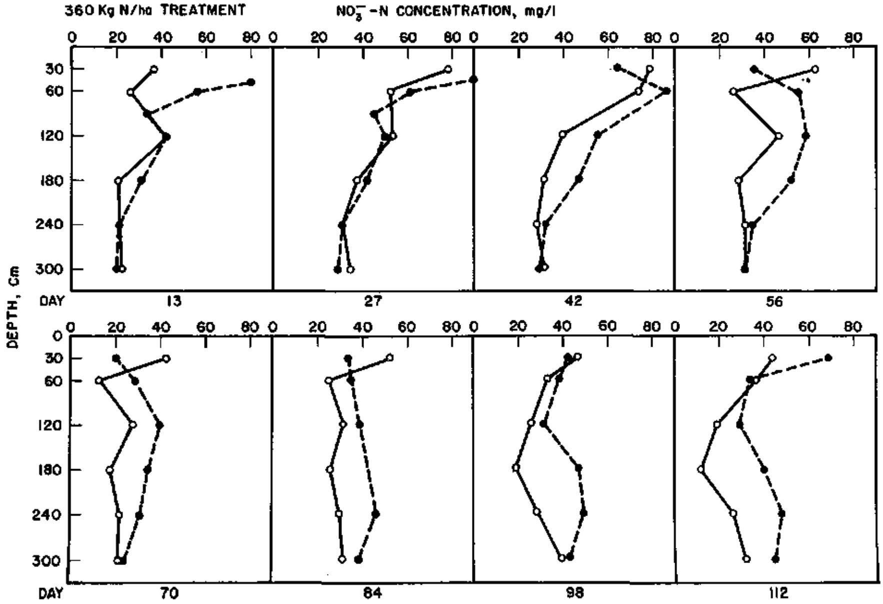


Fig. 10. Measured (solid line) and simulated (broken line) NO_3^- concentration profiles at different days for the 360-kg ha^{-1} N treatment of the 5/3 ET irrigation regime in 1975.

before mentioned limitations were mainly imposed for accuracy relative to checks on mass balance for both water and N.

13. COMPUTER

At the University of California, this model was run on a Burroughs B6700 system, a medium size computer. It has also been run on PRIME 480 system with some modifications in plant uptake at the US Army CRREL, Hanover, New Hampshire by Mehran and Iskandar.

14. PROGRAM LANGUAGE

FORTRAN IV.

15. RUNNING TIME/COST

	Water flow submodel		N flow submodel	
	Quantity	Charge	Quantity	Charge
Processor time (min.)	5.06	$10.12	3.45	$ 7.11
Virtual memory (kilowords/min.)	8.43	$ 0.67	21.12	$ 1.74
Save and buffer memory (kilowords/min.)	18.59	$ 2.97	12.48	$ 2.06
Other costs		$ 7.77		$ 5.46
Total costs		$21.53		$16.37

The before mentioned total costs are based on use of a time-sharing terminal (DecWriter) and for 131 daily outputs for water flow simulation and 9 output dates (0, 13, 26, 42, 56, 70, 84, 98, and 112 days after planting) for N flow simulation.

16. USERS

a. University of California, Davis for the RANN corn field irrigation-fertilization experiment.

b. US Army Cold Regions Research and Engineering Laboratory (CRREL) at Hanover, New Hampshire for simulating land application of secondary treatment municipal wastewater on grass lysimeter plots.

17. DEVELOPER AND PRINCIPAL CONTACTS

Kenneth K. Tanji (for general information)
Department of Land, Air and Water Resources
University of California
Davis, California 95616
USA

Sumant K. Gupta (for specific questions on water flow submodel)
c/o Battelle Pacific Northwest Laboratories
P.O. Box 999
Richland, Washington 99352
USA

Mohsen Mehran (for specific questions on N flow submodel)
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720
USA

REFERENCES

Acevedo, E., 1975. The growth of maize (*Zea mays* L.) under field conditions as affected by its water relations. Unpublished Ph.D. Dissertation, University of California, Davis, 253 pp.

Biggar, J.W., J. MacIntyre, K.K. Tanji, and D.R. Nielsen, 1979. Field investigation of water and nitrate movement in Yolo soil. Ch. 13. In: P.F. Pratt, Nitrate in effluents from irrigated agriculture, Final Report to NSF, University of California, pp. 467-485.

Biggar, J.W., K.K. Tanji, C.S. Simmons, S.K. Gupta, J.L. MacIntyre, and D.R. Nielsen, 1977. Theoretical and experimental observations of water and nitrate movement below a crop root zone. In: J.P. Law, Jr., and G.V. Skogerboe, (Eds.): Irrigation return flow quality mangement, Proceedings National Conference, Colorado State University, Fort Collins, pp. 71-77.

Broadbent, F.E., and A.B. Carlton, 1979. Field trials with isotopes - plant and soil data for Davis and Kearney sites. Ch. 12, In: P.F. Pratt, Nitrate in effluents from irrigated agriculture, Final Report to NSF, University of California, pp. 433-465.

Gupta, S.K., K.K. Tanji, D.R. Nielsen, J.W. Biggar, C.S. Simmons, and J.L. MacIntyre, 1978. Field simulation of soil-water movement with crop extraction. Department of Land, Air, and Water Resources, University of California, Davis, Water Science and Engineering Paper 4013, 121 pp.

Jackson, R.D., J. Reginato, and C.H.M. van Bavel, 1965. Comparison of measured and calculated hydraulic conductivities of unsaturated soils. Water Resources Research 1: 375-380.

Mehran, M., and K.K. Tanji, 1974. Computer modeling of nitrogen transformations in soils. Journal of Environmental Quality 3: 391-396.

Millington, R.J., and J.P. Quirk, 1961. Permeability of porous soils. Transactions Faraday Society 57: 1200-1207.

Nimah, M.N., and R.J. Hanks, 1973. Model for estimating soil water, plant and atmospheric interrelations: I. Description and sensitivity. Soil Science Society of America Proceedings 37: 522-527.

Pratt, P.F., 1979. Nitrate in effluents from irrigated agriculture. Final Report to NSF, University of California, 822 pp.

Ritchie, J.T., and E. Burnett, 1971. Dry land evaporative flux in a humic climate: II. Plant influences. Agronomy J. 63: 56-62.

Simmons, C.S., D.R. Nielsen, and J.W. Biggar, 1979. Scaling of field-measured soil water properties. Hilgardia 47(4): 77-174.

Tanji, K.K., and M. Mehran, 1979. Conceptual and dynamic models for nitrogen in irrigated croplands. In: P.F. Pratt, Nitrate in effluents from irrigated agriculture, Final Report to NSF, University of Caifornia, 16: 555-646.

Thornthwaite, C.W., and J.R. Mather, 1955. The water budget and its use in irrigation. In: US Department Agriculture Yearbook. US Government Printing Office, Washington, DC, pp. 346-357.

4.2 Simulation of soil-water and nitrogen movement

R.J. Wagenet

1. NAME OF MODEL

The model described in this discussion will be referenced by the name NFLUX.

2. SYSTEMS MODELLED

NFLUX is a one-dimensional model designed to be used in the description of upward or downward fluxes of nitrogen within the soil profile. As such, it can be applied on a field or research plot basis where horizontal fluxes of water and solutes are not a consideration. The model is currently structured to transport and transform urea, ammonium, and nitrate.

In order to accomplish this, the processes of urea hydrolysis, nitrification, denitrification and ammonia volatilization are considered. No mineralization of organic matter is modelled. Plant extraction of water and nitrogen during transport and transformation can be included or not depending on the case under consideration. Description of heat transfer has also been included so that temperature effects on nitrogen transformations can be simulated.

3. OBJECTIVE

The current emphasis of the model is in the description of transient nitrogen fluxes in agricultural systems. In the semi-arid western United States we are also concerned with irrigation management and crop production. NFLUX is designed as a tool to be useful in the study of urea, ammonium, and nitrate transport and transformation under field conditions involving these considerations. Specifically we are interested in simulating two cases. First, we are conducting small research plot (6 m x 6 m) studies of the concomitant leaching of fertilizer and salts. NFLUX allows integration of the research results of these intensive studies so that the effects of transient soil water contents and temperature can be related to nitrogen cycling. Second, we are using NFLUX in field studies (40 m x 120 m) of plant growth, nitrogen uptake and nitrogen leaching. Specifically, corn is being grown under several irrigation management and nitrogen fertilizer regimes, with field measurements taken of both plant and soil parameters used in the model. We hope from this data to develop functional relationships between transient soil nitrogen fluxes, plant growth and nitrogen uptake.

4. TIME SCALE

The model increments time based on water content changes (water-fluxes). As water-flux increases, the model uses smaller time steps to minimize possible numerical dispersion. The smallest allowable time increment is 0.024 hr and the largest allowable is 6.0 hr. The model is usually executed for one growing season per run, representing a simulation time of 3600 hrs (150 days). The model can be executed for longer or shorter times as desired.

5. DIAGRAM

NFLUX is a vertical, multicompartment model (Tillotson et al., 1980), with water flow, nitrogen flow, plant growth, and plant uptake linked in a series of sequential steps. The specific processes included and the manner in which they are related is best understood by the following sequence of NFLUX operations.

a. Using water content versus soil-water matric potential data (measured in pressure plate-outflow experiments) and saturated hydraulic conductivity, the soil's pressure heads, water differential capacities, hydraulic conductivities and diffusivities as functions of water content are calculated using the methods of Erh (1972) and Jackson (1972).

b. Time dependent potential evaporation and potential transpiration rates are calculated from potential evapotranspiration data using the methods of Childs (1975).

c. Root growth (maximum depth of rooting, length of rooting per volume increment, and proportion of active roots in a volume increment) is calculated using the method of Davidson et al. (1978).

d. Hydraulic conductivities, time and space averaged, are calculated from the method of Hanks and Bowers (1962).

e. The surface flux is checked. If the actual evaporation does not reach potential evaporation due to soil moisture constraints then the potential transpiration is increased using the method of Childs (1975).

f. Root extraction of water is calculated using the method of Nimah and Hanks (1973).

g. Soil water contents and fluxes are calculated.

h. Soil temperature and heat fluxes are calculated.

i. Transformation rates (first-order kinetics) for the enzymatic hydrolysis of urea, nitrification, and denitrification can be calculated as functions of water content, temperature, or soil chemistry. At present the functional relationships for these calculations are not known, and the rates are therefore assumed to be constants. The values of Wagenet et al. (1977) are used in the examples of section 11 of this discussion.

j. Nitrogen species urea, ammonium and nitrate are sequentially transported and transformed (see Eq. 10-12).

k. Plant uptake of nitrogen is calculated. Ammonium and nitrate solution concentrations are adjusted for plant removal.

l. Crop yield is calculated based on evapotranspiration predicted by the model. The methods used are those of Hanks (1974). The effects of nitrogen fertility on plant growth have not been included.

6. LEVELS

See section 5.

7. GOVERNING EQUATIONS

a. *Soil water flow*

Transient fluxes of water are calculated using a finite difference solution to

$$C(\theta)\frac{\partial h}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial H}{\partial z}\right] + A(z,t) \tag{1}$$

where

h = soil-water pressure head (cm)
t = time (hr)
z = depth, increasing downward from the surface (cm)
$K(\theta)$ = hydraulic conductivity (cm hr^{-1})
H = hydraulic head (cm)
$C(\theta)$ = differential soil-water capacity = $\partial\theta/\partial h$ (cm^{-1})
θ = volumetric water content (dimensionless)
$A(z,t)$ = rate of plant root extraction of water (hr^{-1}) (see Nimah and Hanks, 1973).

Values for the nonlinear coefficients ($K(\theta)$) are obtained using the method presented by Hanks and Bowers (1962). Values for $C(\theta)$ are determined from the slope of the moisture release curve. Using these approaches, and by collecting known and unknowns, a linear equation of the form

$$Ah^j_{i-1} + Bh^j_i + C^j_{i+1} = D \tag{2}$$

can be developed, for each depth boundary, excluding the upper and lower. The coefficients A, B, C, and D are all known. The linear system of equations produced at a given time is solved using the Thomas algorithm (Bruce et al., 1953). The Thomas algorithm solves the system of equations produced by converting the tridiagonal coefficient matrix to an upper triangular matrix and solving for the pressure heads by backsubstitution.

b. *Upper and lower boundary flux of water*

The upper boundary condition can change with time to simulate rainfall, irrigation, or evaporation. Rainfall and irrigation represent positive flux of water and evaporation a negative flux. This surface flux of water (EOR) is incorporated into the numerical solution of the water flow equation. Recalling Darcy's law and numerically approximating it gives

$$\text{EOR} \approx \frac{K^{j-\frac{1}{2}}_{i-\frac{1}{2}}}{\Delta z}\left[\frac{\left[H^{j-1}_{i-1} + H^{j}_{i-1}\right]}{2} - \frac{\left[H^{j-1}_{i} + H^{j}_{i}\right]}{2}\right] \tag{3}$$

where $K^{j-\frac{1}{2}}_{i-\frac{1}{2}}$ is the hydraulic conductivity estimated at half time and depth steps from Hanks and Bowers (1962). Recognizing that there is no (i-1) depth increment at the surface, the value of EOR can be substituted into the differenced form of Eq. (1) to provide an equation of the form of Eq. (2), but pertaining only to the soil surface. At the soil surface A(z,t) is assumed equal to zero.

For the lower boundary condition the model can simulate no flux ($\partial H/\partial z = 0$), a unit hydraulic gradient ($\partial H/\partial z = -1$), a constant soil-water pressure head, and a watertable.

c. *Solute flow*

The diffusion-convection equation for a non-interacting solute is used by NFLUX as the basis for transport of the nitrogen species. This equation is

$$\frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta,q)\,\frac{\partial c}{\partial z}\right] - \frac{\partial}{\partial z}\,(qc) \tag{4}$$

where

c = concentration of solute (mg ℓ^{-1})

$D(\theta,q)$ = apparent diffusion coefficient (cm hr^{-1})

q = water-flux (cm hr^{-1})

and the other terms are as defined above.

In the case of a solute that interacts with the soil surface or has sources and sinks in the soil, Eq. (4) can be modified to:

$$\frac{\partial(\rho s)}{\partial t} + \frac{\partial(\theta c)}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta,q)\,\frac{\partial c}{\partial z}\right] - \frac{\partial}{\partial z}\,(qc) \pm \phi \tag{5}$$

where

ρ = soil bulk density (g cm^{-3})

s = mass of ion adsorbed per mass of soil

ϕ = source or sink of ion (mg ℓ^{-1} hr^{-1}).

The description of nitrogen transport and transformation is accomplished using three equations of the form of Eq. (5). NFLUX first assumes a sequential transformation by first-order kinetics from urea to ammonium to nitrate. That is,

$$\begin{array}{ccccccc} \text{urea} & \xrightarrow{k_1} & \text{ammonium} & \xrightarrow{k_2} & \text{nitrate} & \xrightarrow{k_3} & \begin{array}{l}\text{gaseous}\\ \text{products}\end{array} \\ c_1 & & c_2 & & c_3 & & \end{array}$$

where

c_1 = concentration of urea
c_2 = concentration of ammonium
c_3 = concentration of nitrate.

The kinetics can be written as:

$$\frac{\partial c_1}{\partial t} = -k_1 c_1 \tag{6}$$

$$\frac{\partial c_2}{\partial t} = -k_2 c_2 + k_1 c_1 \tag{7}$$

$$\frac{\partial c_3}{\partial t} = -k_3 c_3 + k_2 c_2 \tag{8}$$

The ions urea and ammonium both undergo interaction with the soil surface that acts to slow their movement through soil. For each of these interactions it was assumed that

$$s_i = R_i c_i$$

where s_i is the mass of ion i adsorbed per mass of soil and R_i is a linear partition coefficient (determined in independent laboratory experiments) relating adsorbed to solution concentrations. Using Eq. (5-9), a series of three solute displacement equations can be written that describe the sequential transformation and simultaneous transport of urea, ammonium and nitrate. That is

$$\frac{\partial(\rho s_1)}{\partial t} + \frac{\partial(\rho c_1)}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta,q)\frac{\partial c_1}{\partial z}\right] - \frac{\partial}{\partial z}(qc_1) - k_1 c_1 \theta \tag{10}$$

$$\frac{\partial(\rho s_2)}{\partial t} + \frac{\partial(\theta c_2)}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta,q)\frac{\partial c_2}{\partial z}\right] - \frac{\partial}{\partial z}(qc_2) - k_2 c_2 \theta + k_1 c_1 \theta \tag{11}$$

$$\frac{\partial(\theta c_3)}{\partial t} = \frac{\partial}{\partial z}\left[D(\theta,q)\frac{\partial c_3}{\partial z}\right] - \frac{\partial}{\partial z}(qc_3) - k_3 c_3 \theta + k_2 c_2 \theta \tag{12}$$

Equations (10), (11) and (12) are solved by finite differencing using methods of Bresler (1973) to calculate $D(\theta,q)$ and to minimize numerical dispersion. An equation of the form of (2) is obtained, which is similarly solved for concentration now instead of soil-water pressure head.

e. *Upper and lower boundary flux of solute*

The solute upper boundary conditions are the solute concentrations in the irrigation or rain water. During evaporation the mass flow and diffusive flow of solute at the surface are assigned values of zero in order to avoid solute flux through the soil surface. The solute lower boundary conditions are assumed equal to constant concentrations measured deep in the soil profile.

f. *Heat flow*

The heat flow equation included in NFLUX is

$$(0.2\ \rho + \theta)\ \frac{\partial T}{\partial t} = \frac{\partial}{\partial z}\left[K_q(\theta)\frac{\partial T}{\partial t}\right] \tag{13}$$

where

ρ = soil bulk density (g cm^{-3})
0.2 = specific heat of soil (cal $g^{-1}{}^{o}C^{-1}$)
T = temperature (^{o}C)
$K_q(\theta)$ = thermal conductivity (cal $cm^{-1}hr^{-1}{}^{o}C^{-1}$)

and the other terms are as were defined above.

Values of $K_q(\theta)$ are calculated using the approximation technique (Hanks and Bowers, 1962) explained earlier in the calculation of hydraulic conductivity.

g. *Upper and lower boundary flux of heat*

The upper boundary conditions for soil-temperatures are calculated from the method presented by Kirkham and Powers (1972). That is

$$T_s = T_a + \gamma\ \sin\left[\frac{2\pi t}{p}\right] \tag{14}$$

where

T_s = temperature at the soil surface (^{o}C)
T_a = 'average' measured temperature at soil surface (^{o}C)
γ = amplitude of sine wave (^{o}C)
p = period of time in hours necessary to complete one cycle of the wave (taken to be 24 hrs)
t = time (hr).

Equation (14) considers sinusoidal variation of surface soil temperature. Measured values of T_a and γ corresponding to appropriate time intervals are provided as inputs. These values are expected to be measured by thermocouple just below the soil surface.

The lower boundary condition is assumed equal to a constant temperature measured deep in the soil profile.

h. *Plant root growth*

Using the root length distribution data of NaNagara et al. (1976) for corn grown under field conditions, Davidson et al. (1978) obtained empirical equations describing root growth by 'curve fitting' measured distributions at selected times during the season. These equations are used in NFLUX. The disadvantage to using these equations is they do not consider environmental effects (i.e. nitrogen fertility, water availability, salt concentration) on root growth. We have been unable to find substantial experimental data pertaining to these points.

i. *Plant nitrogen uptake*

Nye and Tinker (1977) present an equation used in NFLUX to calculate nitrogen uptake. That is

$$I = 2\pi r c \alpha \tag{15}$$

where

I = rate of nutrient uptake per unit length of root (mg $cm^{-1}hr^{-1}$)
r = root radius (cm)
$2\pi r$ = circumference of root (cm)
α = root uptake coefficient or root absorbing power (cm hr^{-1})
c = nutrient concentration in solution during the uptake period (mg ℓ^{-1})

Estimation of the value of α is accomplished using the work of Warncke and Barber (1973). For a study with corn they found that

$$\log \alpha_{NH_4^+} = -6.81 - 0.63 \log (NH_4^+) - 116.8\ (NO_3^-) \tag{16}$$

and

$$\log \alpha_{NO_3^-} = -6.80 - 0.61 \log (NO_3^-) - 127.1\ (NH_4^+) \tag{17}$$

where (NH_4^+) and (NO_3^-) are solution concentrations in moles/liter.

The nitrogen species solution concentrations around the roots during the uptake period are equal to the values predicted by Eq. (10-12). The plant root profile is partitioned according to the volume increments established by the depth boundaries and area associated with each plant. Plant extraction of a nitrogen species from a volume increment cannot exceed the amount of that nitrogen species in that increment.

j. *Ammonia volatilization*

The dry, calcareous soils used in the application of this model exhibit substantial tendency for NH_4^+ loss via volatilization. NFLUX uses a first-order rate constant of 0.3 hr^{-1}, obtained by extrapolating the work of Chin and Kroontje (1963) to dry conditions, to decrease NH_4^+ concentrations in the upper 2 cm of the soil surface.

k. *Mineralization and immobilization*

The process of mineralization and the reverse process of immobilization are not considered in this modelling effort. The experimental cases presented are soils low in organic matter.

8. INPUT PARAMETERS

NFLUX requires the following inputs:

a. Data of volumetric water content versus soil-water pressure for selected points of the moisture release curve (including h = 0 cm and h = -15,000 cm).

b. Depth boundaries.

c. Initial soil conditions at depth boundaries of volumetric water content, urea, ammonium and nitrate concentrations, masses of urea and ammonium, and temperature.

d. Surface boundary conditions of

1. irrigation frequency, duration, rate,
2. concentrations of nitrate and masses of urea and ammonium in each irrigation water increment,
3. rainfall frequency, duration, rate,
4. potential evapotranspiration rates and their appropriate times,
5. average surface soil temperature and duration.

e. The upper and lower limits of soil water pressure and water content (i.e. saturation and air dry).

f. The upper and lower limits of soil water pressure from which plant roots may extract water.

g. Maximum allowed water content change in the soil profile for a time increment.

h. Time to stop calculations (final end time).

i. Urea and ammonium partition coefficients (R_1 and R_2).

j. Functional relationships for nitrogen transformation (if non-constant values of k_1, k_2, and k_3 are desired).

k. Saturated hydraulic conductivity.

l. Soil bulk density.

m. Bottom boundary conditions for water.

n. Crop factors related to plant growth (currently corn).

1. number of days to root profile maturity,
2. number of days to achieve total crop cover,
3. percent of bare soil cover at crop maturity,
4. planting density,

5. nitrogen uptake functions (if different from Eq. 16, 17),
o. Physical constants used in heat transfer (if different from Wierenga et al., 1969).

9. VERIFIABLE OUTPUTS

NFLUX provides as output soil profiles with time of the following potentially measurable parameters:

a. Soil-water pressure heads.
b. Volumetric water contents.
c. Urea concentrations in solution and adsorbed.
d. Ammonium concentrations in solution and adsorbed.
e. Nitrate concentrations in solution.
f. Root distribution.
g. Root water extraction.
h. Root nitrogen extraction.
i. Soil temperature.

Nitrogen content of the plant as a function of time is also calculated.

10. OBSERVATIONS

Experimental design for validation or use of this model is limited to one-dimensional water flow, uniform broadcast application (or incorporation) of nitrogen compounds, and uniform sprinkler or ponding application of water. Data is most readily developed in experiments that are designed to allow soil sampling, soil-water sampling, plant analysis, temperature measurement and water content determinations during the course of the growing season. We have used the line-source, continuous variable irrigation system of Hanks et al. (1976) in conjunction with several rates of nitrogen fertilization in field studies of corn growth and nitrogen. Neutron probes are used to measure water content, soil samples are analysed for urea, ammonium (exchangeable and solution) and nitrate, and plant samples are collected as the growing season progresses. Transient fluxes of water and solutes and nitrogen uptake can be monitored in this design. Temperature measurements have not to date been taken. On the small, intensively monitored plots mentioned in section 3, procedures are adapted to use soil solution suction probes to measure solute concentrations. Periodic, but much less regular, soil samples are taken. In both cases, evaporation pan and rainfall data must be collected.

At present the best available data relating to root growth is that of NaNagara et al. (1976). If destructive sampling of above-ground corn is accomplished for N content, valuable complementary data would be below ground harvest of root systems. At present manpower limitations have prevented the collection of this data.

11. COMPARISON RESULTS

Predictions made by the model have been compared with one set of field data involving the growth of a corn crop over a 120-day period. Planting density was 60,000 plants/ha, with a broadcast nitrogen application of 500 kg/ha as urea. Irrigation was sprinkler applied as eight events totalling 18 cm over the first 105 days of the season. There was also 21 cm of rain. At several times during the season, measurement was made of soil water content and soil solution nitrate concentrations. No measurements were made of urea and ammonium. At harvest, the nitrogen content of the corn was determined.

Comparison between predicted and measured soil-water profiles at selected times during the growing season (time = 0 corresponded to planting) were made using the model with a soil-water bottom boundary condition at 150 cm of a unit hydraulic gradient. Water content was measured with a neutron probe at three sites in the field at each depth. The agreement between measured and predicted soil-water contents was satisfactory for all times during the growing season. This indicated that the differencing techniques used were able to describe transient fluxes of water in the field. Using these same differencing techniques in the solute flow equation was therefore not considered to be a source of any discrepancy between measured and calculated solute values (discussed below).

Measured NO_3^--N concentrations were obtained by taking soil samples at three locations in the field from depth increments of 0-30, 30-60, and 60-90 cm. The NO_3^--N concentrations predicted by the model were averaged over the intervals 0-30, 30-60, and 60-90 cm to

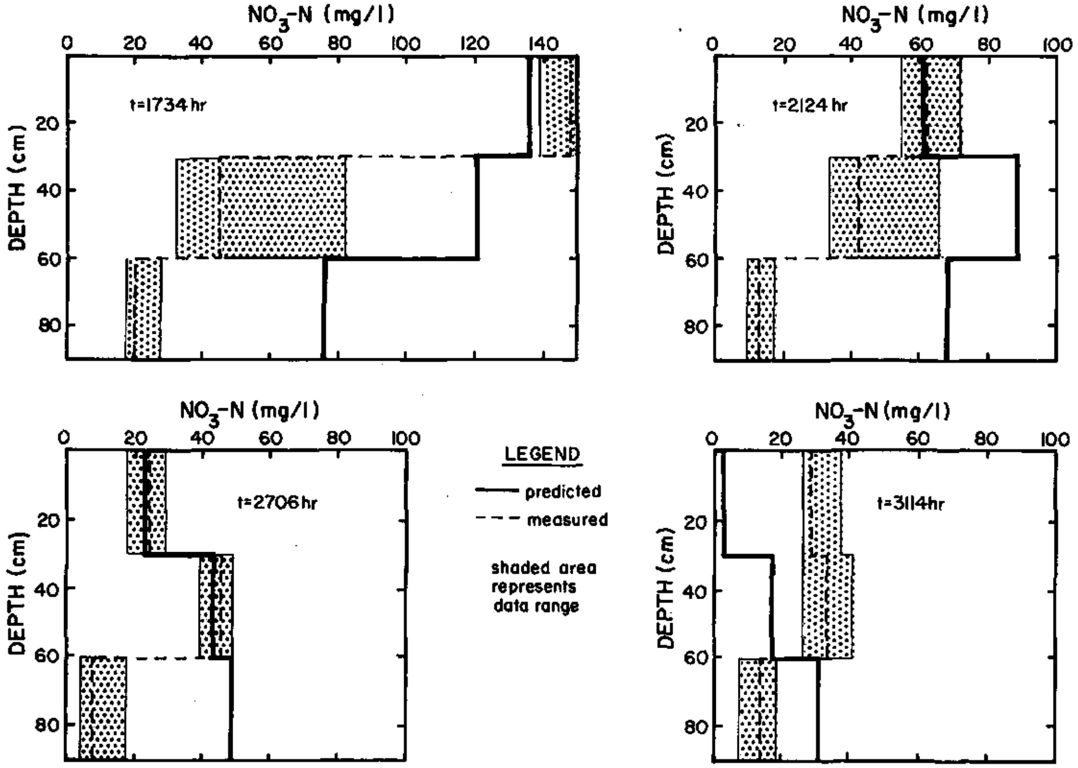


Fig. 1. Comparison of measured and calculated soil solution nitrate concentrations for four times during the season.

obtain average values corresponding to the measured data. The ability of the model to predict the NO_3^--N profiles through a growing season was fair (Fig. 1). There was substantial variation in nitrate values measured in different areas of the field. The use of a single averaged value of NO_3^--N concentration is deceiving as a test of the model's ability to fit observed NO_3^--N concentrations. As more is learned of the spatial variability of nitrate leaching and microbiological processes it is hoped to adapt the modelling procedures. Differences between the range of measured values and the predicted values probably resulted from several assumptions that at this point represent model weakness. These included (1) assuming the nitrogen transformation rates to be constants with depth and time, (2) incorrect partition coefficients for urea and ammonium, (3) incorrect nitrogen species extraction pattern by the crop, or (4) incorrect assumptions about mineralization and immobilization of nitrogen. Measured urea and ammonium soil solution values during transport and transformation were not available in this study but are needed to aid in selecting the proper values for the kinetic nitrogen transformation rates. Further investigation under controlled conditions is also needed to relate values of the rate parameters to dynamic situations of water content, temperature, organic carbon, salts and other pertinent environmental factors. NFLUX is able to maintain a mass balance of nitrogen in the system.

The kinetic transformation rates for urea hydrolysis, nitrification, and ammonium volatilization in this modelling effort resulted in the disappearance of urea and ammonium from the soil by 510 hours after the application of urea. The rate of disappearance of urea and ammonium can be regulated not only by the values of the transformation rates but also by the partition coefficients. The values selected for these parameters as well as the denitrification rate and plant uptake pattern control the NO_3^--N soil solution concentrations. Sensitivity analysis using hypothetical values of the rate coefficients has shown that NO_3^--N soil solution concentrations are quite sensitive to changes in transformation rates used by the model. There therefore exists substantial opportunity to refine our ability to predict transient nitrogen fluxes using this approach.

There is good agreement between the predicted and measured nitrogen content of the corn plants at the end of the season (Fig. 2). The predicted nitrogen uptake pattern by a corn plant is sigmoidal, as is generally accepted to be the nitrogen uptake. It is important to realize that the sigmoidal pattern was not arbitrarily produced as a pre-designed model input. It was, rather, produced as the result of integrating a dynamic nitrogen transport and transformation description with root growth and nitrogen uptake models.

12. LIMITS AND LIMITATIONS

Time steps are variable between 0.024 hr and 6.0 hr. The user has no control over the time step as it is determined by water content changes.

Depth increments should be kept as small as is economically possible. The divided differencing technique used allows for unequal depth increments, but the size of these increments should be 20 cm or less.

The main limitation to program usage is the unknown nature of several functional rela-

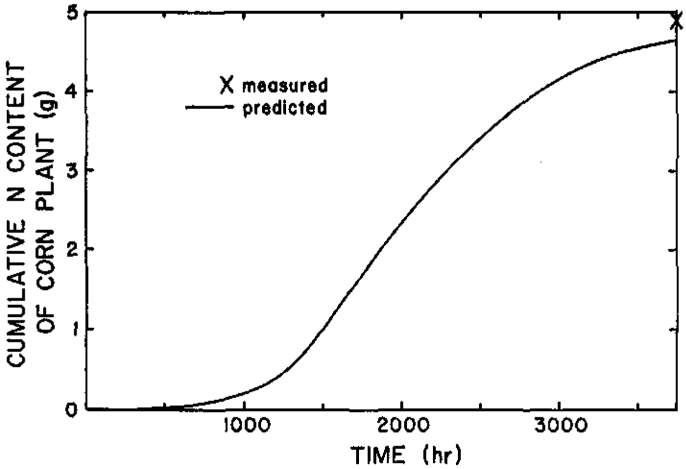


Fig. 2. Comparison of measured and calculated plant uptake of nitrogen.

tionships. We recognize their importance but do not recognize their form. If the user is willing to accept the empirical nature of the present form of these relationships, the model can be used easily. However, the most important further work, in our opinion, needs to be accomplished related to:

a. Relationships between k_1, k_2, k_3 and water content, temperature, organic carbon, and soil chemical properties.

b. The nature of α used in nitrogen uptake routine.

c. The effects of fertility, water management, and soil properties on root and extraction.

d. The importance of volatilization as a sink of applied nitrogen.

13-14. COMPUTER AND PROGRAM LANGUAGE

NFLUX is written in Fortran and is currently executed on a Burroughs 6700. It consists of about 1200 statements.

15. RUNNING TIME/COST

A typical simulation run of 3600 hours of transient fluxes and plant growth involves a CPU time of 420 seconds which on our computer costs about \$31.

16. USERS

At present the model has only been used at Utah State University. It has been designed to be transferable to other situations of climate, soil, and crop, given appropriate inputs.

17. DEVELOPER AND PRINCIPAL CONTACTS

Dr. R.J. Wagenet
Department of Soil Science and Biometeorology
Utah State University
Logan, Utah 84322
USA

REFERENCES

Bresler, E.A., 1973. Simultaneous transport of solutes and water under transient unsaturated flow conditions. Water Resources Research 9: 975-986.

Bruce, G.H., D.W. Peaceman, H.H. Rachford, Jr., and J.D. Rice, 1953. Calculations of unsteady-state gas flow through porous media. Transactions of the American Institute of Mining and Metallurgical Engineers 198: 79-92.

Childs, S.W., 1975. A model to predict the effect of salinity on crop growth. M.S. Thesis, Utah State University, Logan.

Chin, W., and W. Kroontje, 1963. Urea hydrolysis and subsequent loss of ammonia. Soil Science Society of America Proceedings 27: 316-318.

Davidson, J.M., D.A. Graetz, P.S.C. Rao, and H.M. Selim, 1978. Simulation of nitrogen movement, transformation, and uptake in plant root zone. Environmental Protection Agency Report EPA-600/3-78-029. Environmental Research Laboratory, EPA, Athens, Georgia, USA. 106 pp.

Erh, K.T., 1972. Application of the spline function to soil science. Soil Science 114: 333-338.

Hanks, R.J., 1974. Model for predicting plant yield as influenced by water use. Agronomy Journal 66: 660-665.

Hanks, R.J., and S.A. Bowers, 1962. Numerical solution of the moisture flow equation for infiltration into layered soils. Soils Science Society of America Proceedings 26: 530-534.

Hanks, R.J., J. Keller, V.P. Rasmussen, and G.D. Wilson, 1976. Line source sprinkler for continuous variable irrigation-crop production studies. Soil Science Society of America Journal 40: 426-429.

Jackson, R.D., 1972. On the calculation of hydraulic conductivity. Soil Science Society of America Proceedings 36: 380-382.

Kirkham, D., and W.L. Powers, 1972. Advanced Soil Physics. John Wiley and Sons, Inc., New York, New York, USA. 534 pp.

NaNagara, T., R.E. Phillips, and J.E. Leggett, 1976. Diffusion and mass flow of nitrate-nitrogen into corn roots grown under field conditions. Agronomy Journal 68: 67-72.

Nimag, M.N., and R.J. Hanks, 1973. Model for estimating soil water, plant and atmospheric interrelations: I. Description and sensitivity. Soil Science Society of America Proceedings 37: 522-527.

Nye, P.H., and P.B. Tinker, 1977. Solute Movement in the Soil-Root System. Studies in Ecology Series, Volume 4, University of California Press, Berkeley, California, USA, 342 pp.

Tillotson, W.R., C.W. Robbins, R.J. Wagenet, and R.J. Hanks, 1980. Soil-water, solute and plant growth simulation. Utah Agricultural Experiment Station Bulletin No. 502. Utah State University, Logan, Utah, USA. 53 pp.

Wagenet, R.J., J.W. Biggar, and D.R. Nielsen, 1977. Tracing the transformations of urea fertilizer during leaching. Soil Science Society of American Journal 41: 896-902.

Warncke, D.D., and S.A. Barber, 1973. Ammonium and nitrate uptake by corn (*Zea mays* L.) as influenced by NH_4/NO_3 ratio. Agronomy Journal 65: 950-953.

Wierenga, P.J., D.R. Nielsen, and R.M. Hagan, 1969. Thermal properties of a soil based upon field and laboratory measurements. Soil Science Society of America Proceedings 33: 354-360.

4.3 Simulation of nitrogen behaviour in the root zone of cropped land areas receiving organic wastes

P.S.C. Rao, J.M. Davidson and R.E. Jessup

1. NAME OF MODEL

NITROSIM.

2. SYSTEMS MODELLED

Cropped land areas receiving applications of fertilizer N, animal manures and plant residues.

3. OBJECTIVE

Simulation of transport and plant uptake of nitrogen and water and transformations of nitrogen and carbon in the root zone for agricultural fields receiving inorganic fertilizer N, animal manure, and plant residue applications.

4. TIME SCALE

The program is designed to simulate an entire crop growing season (about 120 days). Time resolution for various processes ranges from minutes to hours.

5. DIAGRAM

The model NITROSIM is modular in nature and consists of various submodels, each describing a physical or a biological process (Fig. 1).

7. GOVERNING EQUATIONS

Two principal factors governed the development of NITROSIM. The input parameters necessary for verification and subsequent use must be readily available or at least their values can be estimated from existing data. The model structure must be simple enough to require minimum computational time and yet provide an accurate description of the dynamics of water, nitrogen, and carbon in the root zone. This was accomplished by using various simplified and/or empirical, but conceptually-based, relations in the model. The development and verification of NITROSIM are described in greater detail by Rao et al. (1980).

The primary function of the water transport submodel is to update the soil-water content (θ^i) and soil-water flux (q^i) in each depth increment (i=1,2...n) and also to account for soil-water extraction by plant roots. In this submodel, a simplified approach was used, where water transport was considered to occur in the following three phases: water input (infiltration), water redistribution, and no flow (static). It was assumed that

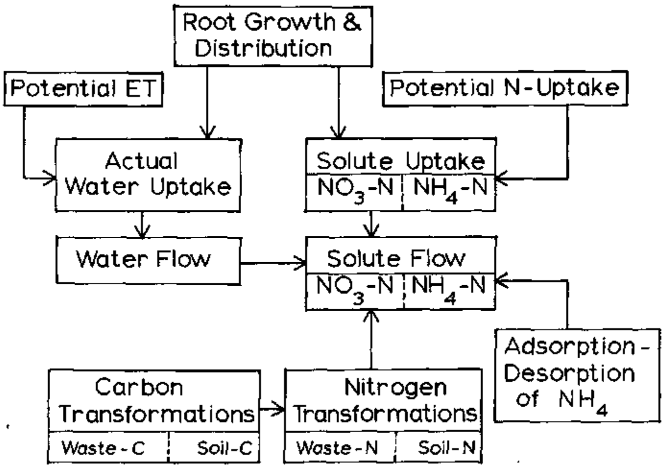


Fig. 1. Flow diagram showing inter-relationships between various processes included in the model NITROSIM.

during a water input phase, water enters the soil surface at a steady flux ($q^1 = q^s$) and increases the soil-water contents in the wetted depth increments to θ^s. Eqs. (1)-(4) state the algorithm for the water input phase:

$$\theta^{i*} = \theta^i + q^i \frac{\Delta t}{\Delta x} - U_w^i \Delta t;\ \theta^{i*} \leqq \theta_s \tag{1}$$

$$\theta^{i*} = \theta^i (t + \Delta t) \tag{2}$$

$$q^1 = q^s \tag{3}$$

$$q^{i+1} = [q^i - \frac{\Delta x}{\Delta t} (\theta^{i*} - \theta^i) - U_w^i \Delta x];\ i \geqq 1. \tag{4}$$

During the water redistribution phase, soil-water contents in the wetted depth increments decrease 'exponentially' to a 'field-capacity' value (θ_{fc}). Water drained from the wetted increments increases the θ of lower depth increments. These depth increments also drain a later time. All calculations are perfomed on the basis of reduced soil-water content (r_i) defined as:

$$r_i = \frac{\theta^i - \theta^i_{fc}}{\theta^i_s - \theta^i_{fc}} \tag{5}$$

$$r_i^* = r_i\ (t + \Delta t) = \frac{\theta^{i*} - \theta^i_{fc}}{\theta^i_s - \theta^i_{fc}} \tag{6}$$

The redistribution phase algorithm can be stated by the following relationships. For the first depth increment (i=1),

$$q^1 = 0 \tag{7}$$

$$r_1^* = \begin{cases} r_1; \ \theta^1 \leqq \theta_{fc}^1 \\ r_1 \exp(-\alpha\Delta t); \ \theta^1 > \theta_{fc}^1 \end{cases} \tag{8}$$

For all other depth increments (i=2,3,...,n),

$$r_i^* = \begin{cases} r_1; \ \theta^i \leqq \theta_{fc}^i, \ r_{i-1}^* \leqq r_i & \text{(10a)} \\ r_1^* \exp(-\alpha\Delta t); \ \theta^i > \theta_{fc}^i; \ r_{i-1}^* \leqq r_i & \text{(10b)} \end{cases}$$

$$\theta^{i*} = \theta^i + q^i \ (\Delta t/\Delta x) \tag{11}$$

$$\theta_{MAX} = \theta_{fc}^i + r_{i-1}^* \ (\theta_s^i - \theta_{fc}^i); \ \theta_i^* \leqq \theta_{MAX} \tag{12}$$

$$q^{i+1} = (\Delta x/\Delta t) \ (\theta^i - \theta^{i*}) + q^i \tag{13}$$

Also, for all increments (i=1,2,...,n), the evapotranspiration losses are accounted as follows:

$$\theta^{i*} = \theta^{i*} - U_w^i \ \Delta t \tag{14}$$

The no-flow phase is reached when in all wetted depth increments $\theta = \theta_{fc}$. During this phase, the only changes in soil-water content are due to plant root extraction. Thus,

$$\theta^{i*} = \theta^{i*} - U_w^i \ \Delta t \tag{15}$$

Transport of water-soluble nitrogen species (NO_3-N and NH_4-N) was assumed to occur only due to convective flow and the contribution of dispersive flow was neglected. Nitrate-N was considered to be non-reactive, while the adsorption (or ion-exchange) of NH_4-N was described by a linear and reversible isotherm. The equation describing transport of NO_3-N and NH_4-N is:

$$[(\rho^i K^i + \theta^{i*}) \ C_k^{i*}] - [(\rho^i K^i + \theta^i) \ C_k^i] = \frac{\Delta t}{\Delta x} \ (q^{i+1} \ C_k^i - q^i \ C_k^{i-1}) \tag{16}$$

By letting $M_t = \rho^i K^i + \theta^i$, and $M_t^* = \rho^i K^i + \theta^{i*}$,

$$C^{i*} = \frac{1}{M_t^*}\left[\frac{\Delta t\, q^i\, C^{i-1}}{\Delta x} - \frac{\Delta t\, q^{i+1}\, C^i}{\Delta x} + M_t\, C^i\right] \tag{17}$$

In Eq. (16), subscripts $k = 3$ and 4 designate, respectively, NO_3-N and NH_4-N. Note that $K^i = 0$ for NO_3-N, whereas $K^i = K_D^i$ for NH_4-N.

The decreases in soil-water contents in each depth increment owing to extraction by plant roots in response to evapotranspiration demands were calculated by the Molz and Remson (1970) model as modified by Davidson et al. (1978). Given the potential evapotranspiration demand (PET), the soil-water extraction term U_w^i is calculated as:

$$U_w^i = (\mathrm{PET})(f_w)\left[\frac{K_s^i\, R_r^i}{\sum_{i=1}^{n_r} K_s^i\, R_r^i\, \Delta x}\right] \tag{18}$$

The factor f_w in Eq. (18) is an empirical function that adjusts PET to actual ET depending upon the soil-water status. The following equations define the f_w function:

$$W_r = \sum_{i=1}^{n_r} (\theta^i - \theta_{15}^i)\, \Delta x \tag{19}$$

$$W_a = \sum_{i=1}^{n_r} (\theta_{fc}^i - \theta_{15}^i)\, \Delta x, \text{ and} \tag{20}$$

$$f_w = W_r/(0.2\, W_a),\ 0 \leq f_w \leq 1 \tag{21}$$

Empirical functions were used to describe nitrogen uptake by plant roots. It was assumed that both NO_3-N and NH_4-N were taken up by plants. Similar to PET in the water uptake submodel, a potential maximum N-uptake demand (Q_x) was estimated. This demand was met only when the crop was neither under water- or nitrogen-stress. The crop was considered to be under N-stress, when the soil solution concentrations of NH_4-N and NO_3-N decreased below a pre-established critical minimum (C_{3m} and C_{4m}). The N-stress factor, f_N, was defined as:

$$f_N = [\Delta x \sum_{i=1}^{n_r} R_r^i\, E_N^i]^{-1};\ E_N^i = E_3^i + E_4^i \tag{22}$$

where,

$$E_3^i = \begin{cases} 0; & C_3^i \leq C_{3m} \\ C_3^i - C_{3m}; & C_3^i > C_{3m} \end{cases} \tag{23a}$$

$$E_4^i = \begin{cases} 0; & C_4^i \leq C_{4m} \\ C_4^i - C_{4m}; & C_4^i > C_{4m} \end{cases} \qquad (23b)$$

The total N-uptake demand (Q_x) was partitioned between NH_4-N and NO_3-N as follows:

$$U_3^i = Q_x \; f_w \; f_N \; R_r^i \; E_3^i \qquad (24a)$$

$$U_4^i = Q_x \; f_w \; f_N \; R_r^i \; E_4^i \qquad (24b)$$

The actual total N-uptake (Q_N) is calculated as:

$$Q_N = (\Delta x) \sum_{i=1}^{n_r} (U_3^i + U_4^i) \equiv Q_x \; f_w \qquad (25)$$

The concentration of NO_3-N and NH_4-N are updated as follows:

$$C_3^{i*} = C_3^i - (U_3^i \; \Delta t/\theta_i); \; C_3^i \geq C_{3m} \qquad (26a)$$

$$C_4^{i*} = C_4^i - \frac{U_4^i \; \Delta t}{(\theta^i + \rho^i \; K_D^i)} \; ; \; C_4^i \geq C_{4m} \qquad (26b)$$

The potential N-uptake demand (Q_x) was calculated on the basis of experimental data for corn (Watts and Hanks, 1978) as follows:

$$3.09937 \; (FGS)^3; \; 0 \leq FGS \leq 0.3 \qquad (27a)$$

FTNU =

$$-0.659 \; FGS + 3.48 \; (FGS)^2 - 0.929 \; (FGS)^3 - 0.898 \; (FGS)^4; \; 0.3 \leq FGS \leq 1.0 \qquad (27b)$$

where, FTNU = (CNU/TNU), FGU = (T/TMAX), and $Q_x = \frac{d}{dT}$ (FTNU).

Note that Eq. (27) represents a sigmoidal cumulative N-uptake curve, where the y-axis is normalized by total seasonal uptake (TNU) and the x-axis is normalized by the length of the growing season (TMAX). Eq. (27) is specific to corn crop and should be replaced by appropriate functions for other crops.

The following equations for describing the changes in root density with soil depth and time were developed using field data for corn reported by NaNagara et al. (1976) and Watts (1978). The maximum rooting depth, R_d, was calculated as:

$$R_d = 150/[1 + \exp \; (6 - 12 \; r)] \qquad (28)$$

where, $r = T/80$. Note that a fully grown root system is established in about 80 days after planting. The root density was assumed to be maximum at the soil surface and decrease linearly with depth. Thus,

$$R_r^i = 0.173 \; [R_d - (i - 0.5) \; \Delta x] \tag{29}$$

Again, Eqs. (28) and (29) are specific for corn crop and should not be used for other crops.

In a soil ammended with organic wastes, the native soil organic matter and the added organic waste contribute to the total soil organic N and C contents. Therefore, in simulating C and N transformations, both these components should be considered. The transformations of waste organic C and N were described primarily based on the papers by Reddy et al. (1980a,b). In our model, waste organic C and N are partitioned into 'available' and 'resistant' fractions. The 'resistant' fractions decompose slowly similar to the soil organic C and N, while the 'available' fractions mineralize rapidly.

The carbon transformations submodel calculates the 'available' carbon content in each depth increment at a given time as follows:

$$C_{mc} = (C/N) \; M_n \tag{30}$$

$$C_{amc} = (f_1 + f_2) \; C_{mc} \tag{31}$$

$$\frac{\partial C_{amc}}{\partial t} = -k_{cj} \; C_{amc} \; g_w, \; j = 1, \; 2 \tag{32}$$

$$\frac{\partial}{\partial t} = [C_{sc} + (1 - f_1 - f_2) \; C_{mc}] = - k_s \; g_w \; [C_{sc} + (1 - f_1 - f_2) \; C_{mc}] \tag{33}$$

$$C_{sac} = 24.5 + 0.0031 \; [C_{sc} + (1 - f_1 - f_2) \; C_{mc}] \tag{34}$$

$$C_{av} = C_{sac} + C_{amc} \tag{35}$$

$$g_w = \begin{cases} 1.666 \; \delta^i; \; 0 \leq \delta^i \leq 0.6 & \text{(36a)} \\ 1.75 - 1.25 \; \delta^i; \; 0.6 \leq \delta^i \leq 1.0 & \text{(36b)} \end{cases}$$

The 'available' carbon content is used as an input in simulating denitrification losses.

The transformations of waste organic-N were described using the following equations: For $(C/N) \leq 23$,

$$T_x = T_m \; [1 - 0.043 \; (C/N)] \tag{37}$$

$$T_s = 0.162 \; (T_m - T_x) \tag{38}$$

For (C/N) > 23,

$$T_x = 0 \tag{39}$$

$$T_s = 0.162\ T_m \tag{40}$$

$$T_d = [\ln\ (C/N) - \ln\ 23]/k_d \tag{41}$$

$$\delta^i = \theta^i/[1.0 - (\rho^i/2.65)] \tag{42}$$

$$g^i_{dw} = \begin{cases} 0/\delta^i \leq 0.783 \\ 1.75\ \delta^i - 1.375;\ 0.783 < \delta^i \leq 0.9 \\ 8.0\ \delta^i - 7.0;\ 0.9 \leq \delta^i \leq 1.0 \end{cases} \tag{43}$$

Note that for wastes with (C/N) > 23, there is no 'available' or 'mineralizable' organic-N (T_x) and all of the applied organic waste is considered to be 'resistant' and is treated identical to soil organic-N. Also, following Stanford and Smith (1972), we assume 16.2% of the soil organic-N to be 'mineralizable'.

Nitrogen transformations considered in this model were: nitrification, mineralization, of soil organic-N to NH_4-N, mineralization of waste organic-N to NO_3-N, immobilization of NH_4-N and NO_3-N to soil organic-N, and denitrification of NO_3-N to gaseous-N ($N_2 + N_2O$). All transformations were considered to follow first-order kinetics. The following equations describe N-transformations in our model:

$$\frac{\partial}{\partial t}\ (\theta C_3) = k_1\theta C_4 - k_2\theta C_3 - \rho\frac{\partial G}{\partial t} + k_m\ N_x\rho \tag{44}$$

$$\frac{\partial}{\partial t}\ (\rho S_4 + \theta C_4) = -\ k_1\theta C_4 - k_4\theta C_4 + k_3\rho\ (N_3 + N_m) \tag{45}$$

$$\rho\frac{\partial}{\partial t}\ (N_s + N_m) = k_2\theta C_3 + k_4\theta C_4 - k_3\rho\ (N_s + N_m) \tag{46}$$

$$\frac{\partial N_x}{\partial t} = -\ k_m\ N_x \tag{47}$$

$$\frac{\partial G}{\partial t} = k_5\ C_{av}\ g_{dw}\ \theta\ C_3 \tag{48}$$

$$S_4 = K_D\ C_4 \tag{49}$$

DEFINITION OF SYMBOLS USED

θ	volumetric soil-water content (cm^3/cm^3)
q^i	soil-water flux into ith increment (cm/h)
x	soil depth, positive downward (cm)

t	time (days)
q^s	infiltration rate or maximum soil-water flux (cm/hr)
U_w	evapotranspiration rate per unit depth (hr^{-1})
r	reduced soil-water content (dimensionless)
θ_{fc}	'field-capacity' soil-water content (cm^3/cm^3)
θ_s	'saturated' or 'infiltration' soil-water content (cm^3/cm^3)
α	empirical time constant (hr^{-1})
C_k	solute concentration (μg N/ml), k = 3 for NO_3, k = 4 for NH_4
K_D	NH_4-N adsorption partition coefficient (ml/g)
ρ	soil bulk density (g/cm^3)
PET	potential evapotranspiration demand (cm/hr)
W_r	available soil-water in the root zone (cm)
W_a	total available soil-water in the root zone (cm)
f_w	empirical constant (dimensionless)
f_N	empirical constant (dimensionless)
C_{3m}	'minimum' nitrate concentration (μg N/ml)
C_{4m}	'minimum' ammonium concentration (μg N/ml)
E_3	'effective' nitrate concentration (μg N/ml)
E_4	'effective' ammonium concentration (μg N/ml)
R_r	root density factor (cm root/cm^3)
E_N	$= E_3 + E_4$
U_3	NO_3 uptake rate [(μg N/cm^2)/(cm/hr)]
U_4	NH_4 uptake rate [(μg N/cm^2)/(cm/hr)]
Q_x	potential maximum N-uptake rate [(μg N/cm^2)/hr)]
Q_N	$= Q_x f_w$, actual N-uptake rate
k_1	nitrification rate coefficient (hr^{-1})
k_2	NO_3 immobilization rate coefficient (hr^{-1})
k_3	mineralization rate coefficient (hr^{-1})
k_4	NH_4 immobilization rate coefficient (hr^{-1})
k_5	empirical constant similar to denitrification rate coefficient [(μg C.hr/g)$^{-1}$]
k_m	manure-N mineralization rate coefficient (hr^{-1})
N_s	readily mineralizable soil organic-N content (μg N/g soil)
N_x	readily mineralizable manure/residue organic-N content, Phase I (μg N/g soil)
N_m	Phase II manure/residue organic-N content (μg N/g soil)
G	gaseous nitrogen species, $N_2 + N_2O$ (μg N/g soil)
S_4	adsorbed NH_4 content (μg N/g soil)
T_m	total manure/residue-N applied (μg N/cm^2)
T_x	total Phase I manure/residue-N (μg N/cm^2)
T_s	total Phase II manure/residue-N (μg N/cm^2)
C/N	carbon/nitrogen ratio of manure/residue applied
t_d	delay time in mineralization of manure/residue-N when C/N > 23 (hrs)
k_d	delay time rate coefficient (hr^{-1})

g_{dw}	empirical factor for adjusting k_5 for water content effect on denitrification rate (dimensionless)
C_{mc}	manure/residue total organic-C content (μg C/g soil)
M_n	manure/residue total organic-N content (μg N/g soil)
C_{amc}	readily available manure/residue organic-C content (μg C/g soil)
f_1	fraction available manure/resitue organic-C in Phase I
f_2	fraction available manure/residue organic-C in Phase II
k_{cj}	organic-C mineralization rate coefficient; j = 1 for Phase I, j = 2 for Phase II (day^{-1})
C_{sc}	total soil organic-C content (μg C/g soil)
C_{sac}	available soil organic-C content (μg C/g soil)
g_w	empirical factor for adjusting k_{cj} and k_s for water content effect of organic-C mineralization rate
K_s	soil organic-C mineralization rate coefficient (day^{-1})
FTNU	fractional cumulative N-uptake by plants
FGS	time for planting as fraction of growth season
T	time for planting (days)
TMAX	number of days from planting to harvest (days)
n	number of depth increments in the soil profile
n_r	number of depth increments in the root zone
δ^i	degree of water saturation (dimensionless)
CNU	cumulative N-uptake by plants (μg N/cm^2)
TNU	total N-uptake by plants by end of season (μg N/cm^2)

8. INPUT PARAMETERS

The water transport submodel requires input values for θ_s, θ_{fc}, and θ_{15} values for all depth increments as well as the initial soil-water contents of the soil profile. Also the values of TRD and q^s should be provided. The initial values of the solution-phase concentrations of NO_3-N and NH_4-N and the ion-exchange coefficients K_D for NH_4-N are required in the nitrogen transport submodel. The soil profile distributions of soil organic-N and -C, the C/N ratio and depth of incorporation of the organic waste, and all the rate coefficients should be provided for the nitrogen and carbon transformations submodels. In the nitrogen uptake submodel, the values of TNU, TMAX, C_{3m}, and C_{4m} are needed. In order to run model NITROSIM, the daily amounts of water (received as irrigation or rainfall) and fertilizer-N inputs should be specified. Also, the depth of incorporation, loading rate, and time of application of the organic waste should be stated. Daily values of the potential evapotranspiration (PET) demand must be provided in a tabular form or can be calculated by a user-supplied submodel.

9. OUTPUT VERIFIABLE VARIABLES

The following variables are calculated as a function of soil profile depth and time: solution-phase concentrations of NO_3-N, NH_4-N, exchangeable NH_4-N concentration, soil organic-N and soil organic-C contents, and 'available' carbon contents.

For each day of the simulation period, the total storage of water and various nitrogen species within the crop root zone as well as the cumulative outflows of water and nitrogen are calculated. Accumulated ET losses and total gaseous N losses due to denitrification are also computed for each day. Thus, sufficient information is provided to prepare detailed balance sheets for water and nitrogen on each day of the simulation period.

10. MODEL VERIFICATION

Watts and Hanks (1978) report data on the amounts and the rates of water and nitrogen losses during a growing season from the root zone of sprinkler-irrigated corn grown on coarse-textured (sandy) soils of Nebraska. Their field study included three levels of irrigation ('low' 0.8 ET, 'medium' 1.15 ET, and 'high' 1.5 ET) and three levels of nitrogen fertilizer application (158, 250, and 324 kg N/ha); the nitrogen fertilizer was either broadcast or was applied through the sprinklers with irrigation. Details of the experimental set up and tables of measured data are available in a report by Fischbach et al. (1977). We have used measured data from selected treatments (medium-N; low, medium, and high irrigation) of this study to verify NITROSIM. End-of-the-season balance sheets for water and nitrogen prepared using Watts-Hanks field data and NITROSIM model simulations agree fairly well (Table 1).

Table 1. Comparison of measured and calculated balance sheets of water and nitrogen at the end of corn growing season.

	0.8 ET		1.15 ET		1.5 ET	
	Meas.1)	Calc.2)	Meas.1)	Calc.2)	Meas.1)	Calc.2)
Water balance (cm H_2O)						
Total input	64.7	64.7	78.8	78.8	94.9	94.9
Initial H_2O in profile	21.4	21.8	20.2	20.6	18.6	18.8
Cumulative ET	60.0	59.1	60.0	59.5	60.0	59.7
Stored in profile (< 150 cm)	16.3	8.9	21.8	18.2	24.1	19.0
Cumulative outflow (> 150 cm)	9.8	18.5	17.9	21.7	29.4	35.0
Nitrogen balance (kg N/ha)						
Fertilizer-N added	250	250	250	250	250	250
Initial mineral-N	58	47	55	55	47	58
Mineralized from organic-N	84	80	84	80	84	80
Cumulative plant uptake	178	219	160	184	153	152
Mineral-N profile (< 150 cm)	38	116	44	52	25	39
Cumulative outflow (> 150 cm)3)	50	42	55	150	122	198
Cumulative outflow (> 150 cm)4)	176		185		203	

1) Experiments of Watts and Hanks (1978).
2) Calculated using model NITROSIM.
3) Calculated from measured water balance and NO_3 concentration in outflow.
4) Calculated from nitrogen balance equation.

Rolston et al. (1978) measured absolute amounts and rates of denitrification from a Yolo loam under field conditions for different constant soil-water contents, organic carbon sources (animal manure or cropped) and soil temperatures. Direct measurement of denitrification in these studies was made by monitoring the gas-flux (N_2O and ^{15}N) under an air-tight cover placed over the soil surface for short time intervals each day. Rolston et al. (1980) also measured amounts and rates of denitrification from cropped (perennial rye grass) Yolo loam field plots receiving three irrigation frequencies. These data from the two California field studies were used to verify the carbon and nitrogen submodels of NITROSIM. Total amounts of denitrification (obtained by integrating gaseous-N flux over time) measured and calculated by NITROSIM for twelve plots that were maintained at constant soil-water contents (soil-water tension of 8, 15, 50 and 70 cm water) agreed well (Table 2). Similarly, good agreement can be found between measured and simulated fluxes of (N_2 + N_2O) from Yolo loam field plots under three irrigation frequencies (Figs. 2 and 3).

Table 2. Comparison of measured and calculated denitrification from Yolo soil field plots maintained at constant soil-water contents.

Carbon and soil-water treatment	Total denitrification (kg N/ha)			
	Summer (23 °C)		Winter (8 °C)	
	measured[1]	simulated[2]	measured[1]	simulated[2]
Manure, h = -8 cm			33	52
Manure, h = -15 cm	218	206		
Manure, h = -50 cm			30	0.2
Manure, h = -70 cm	47	57		
Cropped, h = -8 cm			19	21
Cropped, h = -15 cm	40	47		
Cropped, h = -50 cm			2	0.7
Cropped, h = -70 cm	9	8		
Uncropped, h = -8 cm			0.4	3
Uncropped, h = -15 cm	10	15		
Uncropped, h = -50 cm			0.4	0
Uncropped, h = -70 cm	4	2		

[1] Data of Rolston et al. (1978).
[2] Simulated using NITROSIM.

12. LIMITS and LIMITATIONS

The model was designed to provide a field-scale simulation of nitrogen and water behaviour in the crop root zone. Although much more refined 'research-level' models can be devised (see Davidson et al., 1978), their verification and use is limited owing to lack of values for input parameters. Thus, the 'hybrid' model described here (NITROSIM) was developed as a compromise between complete empiricism and a totally mechanistic approach. Most input parameters required in NITROSIM can be easily obtained. NITROSIM was designed for well-drained soils. Hence, soil profiles with impeding layers that result in perched

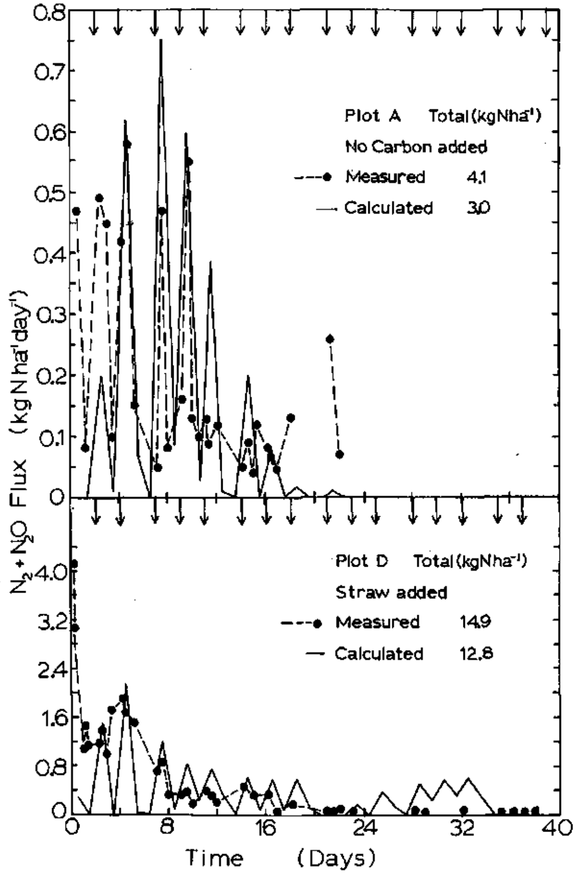


Fig. 2. Measured and calculated surface fluxes of denitrification products (N_2 + N_2O) as a function of time for Yolo soil field plots with and without straw incorporation. The irrigation frequency was three per week. The solid lines are simulated using NITROSIM, while the dashed lines simply connect measured data points. Arrows indicate irrigations.

water tables or tiled-drained soils cannot be simulated with this model. However, water and nitrogen dynamics in non-homogeneous and layered profiles can be described using NITROSIM by specifying different parameter values for each soil depth increment. The N-uptake, ET, and root growth submodels are designed for corn. For other crops, appropriate submodels should be substituted.

13. COMPUTER

Amdhal 470 V/6-11 OS/MVS computing system which is software-compatible with IBM 360/370 systems.

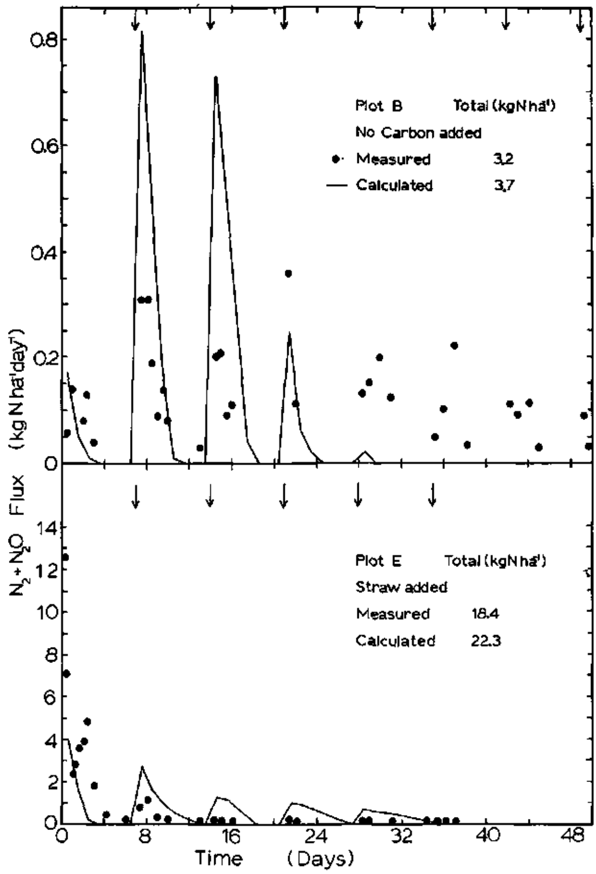


Fig. 3. Measured and calculated surface fluxes of denitrification products ($N_2 + N_2O$) as a function of time for Yolo soil field plots with and without straw incorporation. The irrigation frequency was one per week. The solid lines are simulated using NITROSIM. Arrows indicate irrigations.

14. PROGRAM LANGUAGE

FORTRAN IV G Level 21.

15. RUNNING TIME & COST

0.18 CPU minutes processor time; Cost: $2.00 for simulating 122-day growing season.

16. USERS

The program has been supplied to:

a. Dr. Wynn Walker, Dept. of Agr. & Chem. Engg., Colo. State Univ., Ft Collins, Colorado 80521.

b. Dr. M.R. Overcash, Dept. of Agr. & Biol. Engg., North Carolina State Univ., Raleigh, North Carolina.

c. Dr. D.R. Rolston, Dept. of Land, Air, and Water Resources, Univ. California-Davis, Davis, California.

All three are using our model for simulating the fate of nitrogen in cropped land areas to which either animal manure or crop residues had been applied. Dr. Walker reprogrammed NITROSIM to run on a HP-minicomputer.

17. DEVELOPERS AND PRINCIPAL CONTACTS

P. Suresh Chandra Rao, James M. Davidson, and Ronald E. Jessup
2169 McCarty Hall, Soil Science Dept., IFAS,
University of Florida, Gainesville, FL 32611
USA

ACKNOWLEDGEMENTS

This research was supported by grant No. R-803607 from the US Environmental Protection Agency. The authors are indebted to Dr. K.R. Reddy (University of Florida), Dr. D.G. Watts (University of Nebraska), and Dr. D.E. Rolston (University of California-Davis) for helpful discussions and for providing the data used in NITROSIM development and verification.

REFERENCES

Davidson, J.M., D.A. Graetz, P.S.C. Rao, and H.M. Selim, 1978. Simulation of nitrogen movement, transformation, and uptake in plant root zone. USEPA Ecological Research Series Report. EPA-600/3-78-029. 106 pp.

Fischbach, P.E., D.G. Watts, B.R. Somerhalder, and D.E. Smika, 1977. Protection of a unique ecological area through improved water and fertility management. Technical Completion Report, Water Resources Center, University of Nebraska, Lincoln, Nebraska, 187 pp.

Molz, F.J., and I. Remson, 1970. Extraction-term models of soil-moisture use by transpiring plants. Water Resources Research, 6: 1346-1356.

NaNagara, T., R.E. Phillips, and J.E. Leggett, 1976. Diffusion and mass-flow of nitrate-nitrogen into corn roots grown under field conditions. Agronomy Journal, 68: 67-72.

Rao, P.S.C., J.M. Davidson, R.E. Jessup, and K.R. Reddy, 1980. Simulation of nitrogen behavior in cropped land areas receiving organic wastes. US Environmental Protection Agency Project Report (in press).

Reddy, K.R., R. Khaleel, M.R. Overcash, and P.W. Westerman, 1980a. A nonpoint source model for land areas receiving animal wastes: I. Mineralization or organic nitrogen. Transactions of American Society of Agricultural Engineers, 22: 863-874.

Reddy, K.R., R. Khaleel, and M.R. Overcash, 1980b. Carbon transformations in the land areas receiving organic wastes in relation to nonpoint source pollution: A conceptual model. Journal of Environmental Quality, 9: 434-442.

Rolston, D.E., D.L. Hoffman, and D.W. Toy, 1978. Field measurement of denitrification:

I. Flux of N_2 and N_2O. Soil Science Society of America Journal, 42: 863-869.

Rolston, D.E., A.N. Sharpley, D.W. Toy, D.L. Hoffman, and F.E. Broadbent, 1980. Denitrification as affected by irrigation frequency of a field soil. EPA-600/2-80-066, April 1980, 58 pp.

Stanford, G.S., and S.J. Smith, 1972. Nitrogen mineralization potentials of soils. Soil Science Society of America Journal. 36: 465-472.

Watts, D.G., 1978. Personal Communication.

Watts, D.G., and R.J. Hanks, 1978. A soil-water-nitrogen model for irrigated corn on sandy soils. Soil Science Society of America Journal, 42: 432-499.

4.4 WASTEN: A model for nitrogen behaviour in soils irrigated with liquid waste

H.M. Selim and I.K. Iskandar

1. NAME OF MODEL

WASTEN

2. SYSTEMS MODELLED

This model was developed to describe the N behaviour in land treatment systems as affected by physical, chemical and biological processes and environmental conditions. The model is also capable of describing the fate of N in the soil profile during the growing season of agricultural crops. The region considered is a one-dimensional homogeneous or multi-layered (stratified) soil profile bounded at some depth by an impervious layer, a water table, or extends to a great depth.

3. OBJECTIVE

The objectives of developing the model were:

1. To simulate the physical, chemical and biological processes of N transformation and transport in multi-layered soil profiles irrigated with wastewater under slow and rapid infiltration conditions.
2. To enable prediction of NO_3^--N concentration in soil solution and leachate with time and space.
3. To assist in estimating the application rate and schedule of water and N to a land treatment system.

4. TIME SCALE

The model is flexible and can be used to predict the distribution of N species and N transformations and plant uptake for a part of a growing season. Time resolution is specified by the convergence criteria for individual soils and boundary conditions.

5. DIAGRAM

Figure 1 is a block diagram of the simplified N-model. In addition to the N model, a water flow model describes wastewater infiltration, water movement in each layer of the soil profile, and rate of plant uptake of water with soil depth and time was used. The nitrogen model describes the transport and transformations of N species in each layer of the soil as well as N uptake by plants. The water and N-models include several subroutines for initial and boundary conditions, plant root distribution, soil water properties, and

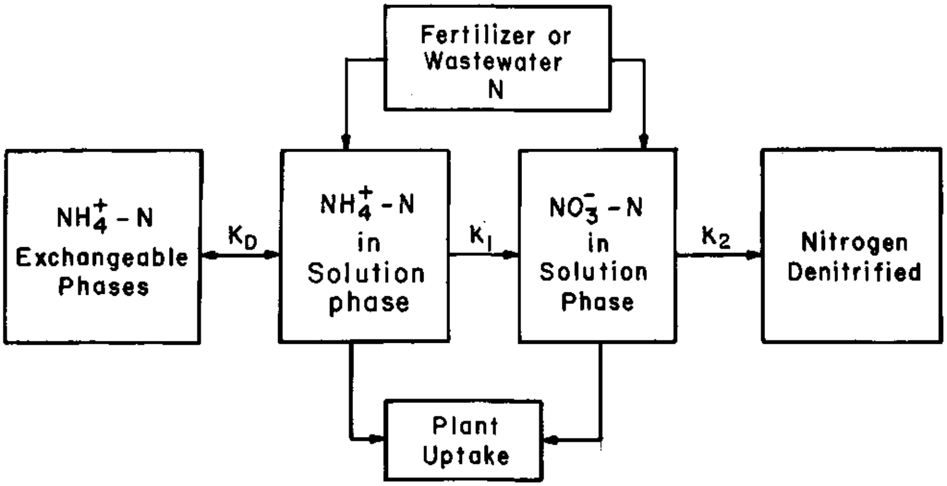


Fig. 1. Schematic diagram of the N-transformation processes considered in the N-model.

nitrogen transformation processes (ion-exchange, nitrification and denitrification).

6, 7. NITROGEN TRANSFORMATION AND TRANSPORT EQUATIONS AND BOUNDARY CONDITIONS

In the development of this model, three major approximations were made. First, the nitrification process was considered as a single step, ($NH_4^+ \rightarrow NO_3^-$) rather than a two step process ($NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$). Such an assumption is considered adequate, since in most soils, under neutral pH conditions, NO_2^- is rapidly oxidized to NO_3^-. Second, the organic-N phase was not incorporated in the model. It was assumed that the net change in organic-N content over a short period of time is small and/or the rates of nitrogen mineralization and immobilization are extremely slow. Third, oxygen diffusion in the soil profile was not incorporated. Therefore, denitrification of nitrate in the soil was assumed to be a function of the degree of soil water saturation only.

The nitrogen transformation processes considered were: nitrification of NH_4^+ to NO_3^-, denitrification of NO_3^-, and ion-exchange of NH_4^+ (see Fig. 1). The ion-exchange process was assumed to be instantaneous, whereas the nitrification and denitrification processes were of the first-order kinetic type (Selim et al. 1976, Selim and Iskandar 1978). A distribution coefficient K_D (cm^3 g^{-1}) was used to describe the instantaneous (reversible) ammonium release from exchange sites to the soil solution. The first-order kinetic (irreversible) rate coefficients associated with the nitrification and denitrification processes were k_1 and k_2 (hr^{-1}), respectively. The assumptions that these N transformation processes follow first-order kinetic reaction were based on studies by McLaren (1970, 1971), Mehran and Tanji (1974), and Hagin and Amberger (1974).

Soil environmental conditions such as soil suction, aeration, temperature, organic matter content, and pH have significant effects on N transformation mechanisms. To incorporate these factors, the rate coefficients were expressed as (Selim et al. 1976).

$$k_1 = \bar{k}_1 f_1,$$

$$k_2 = \bar{k}_2 f_2,$$

where $\bar{k}_1$ and $\bar{k}_2$ are considered constants for each individual soil layer and f_1 and f_2 are empirical functions which describe the influence of the environmental conditions on nitrification and denitrification rate coefficients, respectively.

The transport of NH_4^+-N and NO_3^--N in the soil solution occurs as a result of molecular diffusion, mechanical dispersion, and convection or mass flow. Molecular diffusion results from the random thermal movement of molecules, whereas mechanical dispersion results from the velocity distribution of water in the soil pore space. For all soil layers a single dispersion coefficient D is commonly used which combines mechanical dispersion and diffusion. Therefore, the convective-dispersive equations governing NH_4^+-N and NO_3^--N transport may be expressed as (Misra et al. 1974, Selim et al. 1976, Selim and Iskandar 1978):

$$\frac{\partial(\theta C)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial C}{\partial z}\right) - \frac{\partial(vC)}{\partial z} - \theta k_1 C - \rho \frac{\partial S}{\partial t} - q_{NH_4} \tag{1}$$

$$\frac{\partial(\theta Y)}{\partial t} = \frac{\partial}{\partial z}\left(\theta D \frac{\partial Y}{\partial z}\right) - \frac{\partial(vY)}{\partial z} + \theta k_1 C - \theta k_2 Y - q_{NO_3} \tag{2}$$

where

θ = soil water content ($cm^3\ cm^{-3}$)
z = soil depth (cm)
t = time (hr)
C = concentration of NH_4^+-N in soil solution ($\mu g\ N\ cm^{-3}$)
Y = concentration of NO_3^--N in soil solution ($\mu g\ N\ cm^{-3}$)
D = solute dispersion coefficient ($cm^2\ hr^{-1}$)
v = Darcy's water-flux ($cm\ hr^{-1}$)
S = amount of NH_4^+-N in exchangeable phase per gram soil ($\mu g\ g^{-1}$)
ρ = soil bulk density ($g\ cm^{-3}$)
k_1 and k_2 = kinetic rate coefficients for nitrification and denitrification (hr^{-1}), respectively
q_{NH_4} and q_{NO_3} = rate of plant uptake of NH_4^+-N and NO_3^--N per unit soil volume ($\mu g\ cm^{-3} hr^{-1}$).

The first two terms on the right hand sides of Eq. (1) and (2) account for solute transport, and are usually referred to as the dipersion and mass flow terms, respectively. The third and fourth terms of Eq. (1) account for nitrification and ion-exchange of NH_4^+-N, respectively. Similarly, the third and fourth terms of Eq. (2) represent the nitrification and denitrification processes, respectively. The ion-exchange process governing NH_4^+-N adsorption-desorption was assumed to be of the linear Freundlich type, i.e.

$$S = K_D C \quad \text{or} \quad \partial S/\partial t = K_D\ \partial C/\partial t \tag{3}$$

where K_D, the distribution coefficient ($cm^3\ g^{-1}$), represents the ratio between NH_4^+-N adsorbed and NH_4^+-N in the soil solution. The terms q_{NH_4} and q_{NO_3} are sink terms accounting for root uptake of NH_4^+-N and NO_3^--N.

Rearrangements of Eq. (1) and incorporation of Eq. (3) yield a simplified equation for ammonium transport and transformation:

$$R\partial C/\partial t = D\ \partial^2 C/\partial z^2 - (V/\theta)\ \partial C/\partial z - k_1\ C - (q_{NH_4}/\theta) \tag{4}$$

where R is the retardation factor for ammonium exchange:

$$R = 1 + \rho K_D/\theta \tag{5}$$

and V is expressed as

$$V = v - D\ \partial\theta/\partial z \tag{6}$$

Similarly, Eq. (2), after rearrangements, yields an equation for nitrate transport and transformations:

$$\partial Y/\partial t = D\ \partial^2 Y/\partial z^2 - (V/\theta)\partial Y/\partial z + k_1 C - k_2 Y - (_{NO_3}/\theta) \tag{7}$$

In the case of multi-layered soil profiles, soil water and nitrogen transformation parameters ($\theta(h)$, ρ, $K(h)$, K_D, k_1, k_2, etc.) must be provided for each soil layer.

Prior to solving the NH_4^+-N and NO_3^--N transport and transformations Equations (1) and (2), the water flow equation for multi-layered unsaturated soils must be solved. For one-dimensional unsaturated flow in the multi-layered soil profile the water flow equation (in the I-th layer) is

$$\frac{\partial\theta_I}{\partial t} = \frac{\partial}{\partial z}\left(K_I \frac{\partial h_I}{\partial z}\right) - \frac{\partial K_I}{\partial z} - A(z,\theta),\ (0 < z < L_1) \tag{8}$$

where (omitting the I)

h = soil water pressure head (cm)
K = K(h), soil hydraulic conductivity (cm/hr)
A(z,θ) = soil water extraction ($cm^3\ cm^{-3}\ hr^{-1}$).

To solve the NH_4^+-N and NO_3^- transport and transformation equations simultaneously with the water flow equation (Eq. (4), (7), and (8)), the initial and boundary conditions must be specified. In this model the boundary condition at the soil surface for the water flow equation was considered to be either a water-flux (position for infiltration) or a water heat type boundary condition. For the NH_4^+-N and NO_3^--N equation a third type of boundary condition was chosen at the soil surface. For the bottom boundary condition, a water table at some depth in the soil profile was considered.

Water and nitrogen uptake by plants

Plant uptake of water and nitrogen is an important factor in the renovation of wastewater applied to soil. Recent studies have shown that in a slow infiltration land treatment system, a major portion of the applied wastewater N (up to 70%) was taken up by plants (Iskandar et al. 1976, Palazzo and McKim 1978). Therefore, in modelling the rate of nitrogen in soil it is important to incorporate a plant uptake model that accurately predicts the rate of plant uptake during the growing season. However, as Nye and Tinker 1977) pointed out, the major difficulties in modelling plant uptake of nutrients are the lack of quantitative measurements of root development and distribution and the inaccuracy of soil physical measurements.

There are two approaches to modeling plant root uptake of water and nutrients in soils: a 'microscopic' approach, where the water and nutrient flux to a single root is considered (Nye and Marriot 1969, Claassen and Barber 1974) and a 'macroscopic' approach, where the entire root system as a whole is considered (Molz and Remson 1970, Davidson et al. 1977, Selim and Iskandar 1978). In this model the macroscopic approach is used to describe the water as well as the N uptake by plant roots. The extraction or sink term $A(z,\theta)$ for water uptake (Eq. (8)) was represented as

$$A(z,\theta) = E\ R(z)\ K(h)\ /\ \int_0^L R(z)\ K(h)\ dz \tag{9}$$

where L is the maximum depth of the root zone (cm) and E is the evapotranspiration rate per unit area of soil surface ($cm\ hr^{-1}$). The term R(z) is the root distribution as a function of depth in the soil profile. Specifically, the root distribution R(z) is the length of the roots (cm) as a function of soil depth. Equation (9) was proposed by Molz and Remson (1970) as an empirical approach and was successfully used in predicting the water uptake when the evapotranspiration rate T was met. Such conditions are satisfied when high soil water contents (low suctions) are maintained in the soil root zone, such as in slow infiltration land treatment systems.

In order to account for the effect of the effect of the plant water uptake term on solute concentration, the NH_4^+-N and NO_3^--N concentrations in the soil solution were adjusted such that

$$Y = Y'\ \theta/(\theta - A(z,\theta)\ \Delta t) \tag{10}$$

and

$$C = C' \, (\theta + \rho K_D)/(\theta + \rho K_D - A(z,\theta) \, \Delta t) \tag{11}$$

where C' and Y' are the ammonium and nitrate concentrations before adjustments to changes in soil water content due to water uptake. These adjustments were carried out at every time step, Δt, and were necessary in order to maintain a mass balance of each nitrogen species in the soil matrix.

The terms q_{NH_3} and q_{NO_4} in Eqs. (4) and (7) account for the rate of uptake of NH_4^+-N and NO_3^--N. Here the Michaelis-Menten approach was used to determine the rate of N uptake as a function of root density and concentration of ammonium and nitrate in the soil solution. Therefore the rate of N uptake may be expressed as

$$q_{NH_4} = \frac{I_{max} \, C}{K_m + (C + Y)} \tag{12}$$

$$q_{NO_3} = \frac{I_{max} \, Y}{K_m + (C + Y)} \tag{13}$$

In Eqx. (12) and (13), I_{max} is the maximum rate of N uptake per unit root length (μg hr^{-1} cm^{-1}) when the concentration of nitrogen in the soil solution is extremely high, and the term K_m is the Michaelis constant (μg ml^{-1}), which is the concentration of N at 1/2 I_{max}. Both I_{max} and K_m are determined by measuring N uptake in solution cultures having different N concentrations (Claassen and Barber 1974). In this model the values of I_{max} and K_m were considered similar for both ammonium and nitrate uptake (Barber, personal communication).

8. INPUT PARAMETERS

The main feature of the computer program is that it is valid for uniform as well as multi-layered or stratified soil profiles. In addition, the program is flexible and is designed to incorporate the following (input) conditions as desired:

1. Rate of wastewater application, cm $week^{-1}$
2. Duration of wastewater application, h
3. Depth of individual soil layers, cm
4. Concentration of ammonium and nitrate in the wastewater, μg N ml^{-1}
5. Wastewater application cycly, i.e. scheduling, h
6. Soil water properties and nitrogen transformation mechanisms for individual soil layers
7. Plant root distribution and growth
8. Rate of nitrogen uptake by plants, μg cm^{-1} roots h^{-1}
9. Evapotranspiration rate, cm h^{-1}
10. Initial distribution of soil water and N species in soil solution with depth.

9. OUTPUT

1. Soil water-flux and soil water content at any specified depth and time
2. Cumulative plant water uptake
3. Cumulative water percolated with time
4. Plant uptake of NH_4^+ and NO_3^--N with time
5. Concentration of NH_4^+-N and NO_3^--N in soil solution with depth and time
6. Total amounts of NH_4^+ and NO_3^- leached to the water table.

10. OBSERVATIONS

A lysimeter 91 cm in diameter, and 183 cm high was used to conduct the experiment for model evaluation. Complete discription of the lysimeter and access holes for sample collection is presented elsewhere (Iskandar and Nakano, 1978). The soil used was a Windsor sandy loam soil. The soil profile was 150 cm deep, with A, B and C horizons 15, 30 and 105 cm thick respectively. A water table (zero water pressure head) was assumed at the bottom (150 cm depth) of the soil profile. The soil water properties for each soil layer were described by mathematical expressions which provided 'best fit' of experimental data (Iskandar et al., 1979).

Plant root distribution (R(z)) was assumed to be in the form of an exponential expression

$$R(z) = 226 \exp(-0.1\, z) \tag{14}$$

This empirical relation was obtained from a field study conducted on the same soil under field conditions (Iskandar et al., unpublished data). Total root length per sample area was 2260 cm cm^{-2}. However, some 78% of the roots were present in the top 15 cm, 17% of the roots in the 15-30 cm layer, and only 5% of the roots at 30-60 cm.

Wastewater was applied at a constant flux of 0.38 cm h^{-1} for a period of 10 hours. The evapotranspiration rate (E) was 0.5 cm day^{-1}. The E was considered constant at all times and was calculated from the water balance from several wastewater cycles. No attempts were made to change E with plant age or clippings.

The schedule of wastewater application, the amounts applied each cycle and the concentration of NH_4^+- and NO_3^--N used for model simulation were those of the experimental data. They were calculated every 0.01 hour during infiltration and then successively increased to a maximum time increment of 2 hours during water redistribution.

The N transport and transformation processes considered in the model are those described earlier. For the nitrification kinetic reaction, the function f_1 which describes the dependence of the reaction on soil environmental conditions was expressed as a function of pressure head (Hagin and Amberger 1974).

The denitrification rate was considered to be very small, in the order of 0.01 h^{-1}. Separate experiments on the same soils have confirmed this (Jacobson and Alexander 1978, Iskandar et al. 1976). Plant uptake of N was assumed to follow the Michaelis-Menten equation and was considered to be 0.0005 μg N cm^{-1} roots h^{-1}. The change in root length during the experiment was assumed to be very small and was not accounted for. The maximum specific uptake rate was taken as 1.0 μg ml^{-1}.

The forage grass was clipped and removed from the lysimeters on days 14, 28, 42, 56, 70, 84, 112, 126 and 140 of the experiment.

11. COMPARISON RESULTS

a. *Evaluation of water flow model*

Comparison between model prediction of soil water tension as a function of time after wastewater application with several experimental measurements (Iskandar and Selim, 1981) showed adequate agreement between model prediction and measured soil-water pressure (data not presented).

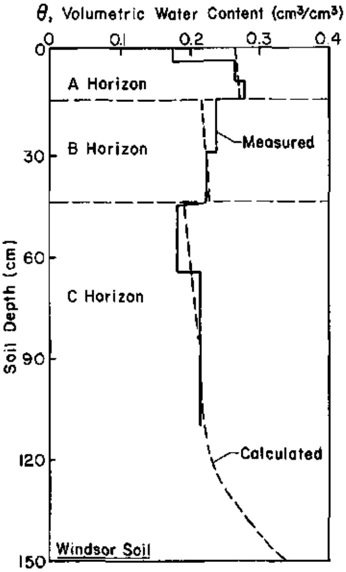


Fig. 2. Comparison between model prediction and experimental data of a soil water content with depth for Windsor soil (Iskandar and Selim, 1981).

Figure 2 shows the measured and calculated soil water content with depths 4 days after application of 3.8 cm of wastewater. Measured soil water contents with depth were obtained gravimetrically. Comparison between measured and calculated results were carried out for both Windsor and Charlton soils (Fig. 2 shows Windsor soil only). Good agreement between model prediction and experimental data was obtained for both soils.

Therefore, from the predictions of the soil water pressure as well as the soil water content distributions with soil depth, the water flow model was considered to be valid. Validation of the water flow model is a prerequisite to describing nitrogen transport in the soil profile.

b. *Evaluation of plant uptake submodel*

To validate the plant uptake submodel, cumulative plant uptake of N from the two soils (Windsor) was compared with model prediction.

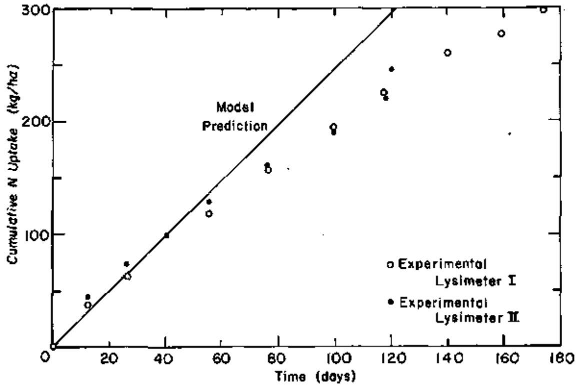


Fig. 3. Comparison between model prediction of plant uptake of N and experimental data.

Figure 3 shows the cumulative plant uptake of N from the two soils compared with model predictions for the Windsor soil. Plant uptake of N was similar for both soils, probably due to the abundance of N in the soil root zone at all times. Since both soils received the same treatments of wastewater (quantity and scheduling) and the cumulative uptake with time is fairly linear, we conclude that the rate of N uptake was constant with time under the controlled experimental conditions of this study.

However, the model slightly overestimated plant uptake of N after 60 days. It seems that actual plant uptake of N decreased slightly with time after 60 days; probably due to higher than optimum temperatures during July and August. Greenhouse studies showed that maximum uptake of N by those grasses occurred at 25 °C. During summer months the greenhouse temperature reaches as high as 35 °C. The maximum difference between model prediction and experimental data was 40 kg N ha^{-1}, which occurred at about 120 days and did not exceed 15% of the cumulative measured N uptake.

Model prediction of plant uptake could probably be improved if plant physiological parameters such as the effect of clipping on root uptake characteristics, uptake of NH_4^+ vs NO_3^- with time, and morphological root characteristics were included in the N prediction. The fact that the plants were a mixture of three different species of forage grass having different morphological and physical characteristics may also account for the small discrepancies between predicted and measured plant N uptake with time.

c. *Distribution of NH_4^+ and NO_3^- in soil solution*

Experimental data showed that NH_4^+-N in soil solution was very low at all soil depths. The maximum concentrations of NH_4^+-N is soil solution in both soils did not exceed 1 μg N ml^{-1} at 7.5 cm depth even 0.5 day after wastewater application. This implies that applied NH_4^+ was removed largely by the soil matrix as well as by plant roots. Sorbed NH_4^+ was then slowly released.

The model, however, predicted much higher concentrations of NH_4^+ in soil solution than were measured (data not presented). As much as 6 μg NH_4^+-N ml^{-1} in soil solution was predicted at depths near the soil surface during the first day of application. However, this decreased rapidly with time. The model also prediced no NH_4^+-N below 15 cm depth at any time.

Figure 4 compares experimental data for soil solution NO_3^- and prediction. For all cases, model predictions showed that fluctuation in NO^--N concentration with time was pronounced at shallow soil depths (7.5 and 15 cm). These fluctuations were mainly due to the frequency of wastewater application as well as to the forms and amounts of N in the wastewater effluent. Such changes in NO_3^--N concentration decreased gradually with soil depth.

It is important to emphasize that varying the $\bar{K}_I$ and K_D values for individual soil layers did not influence the model predictions. This is due to the fact that, for all cases considered, applied NH_4^+-N did not penetrate beyond the first soil layer (15 cm).

With the exception of the sharp peaks at 30 and 150 cm depth, model prediction (Fig. 4) agreed reasonably well with the experimental data. Furthermore, better agreement was obtained with increasing time (after 60 days). The discrepancies between model prediction and the experimental data were probably due to the simplifying assumptions inherent in the model. The model did not include the influence of grass harvesting, during the time period considered, on N-uptake or on root density and distribution. In addition I_{max} was considered constant at all times. The influence of temperature changes on nitrification was also not included in the model. Nor did the model include nitrogen immobilization and mineralization processes. In view of the above simplifying conditions, it is reasonable to conclude that model predictions of NO_3^--N were adequate.

12. LIMITS AND LIMITATIONS

Time and space steps are dictated by the convergence criteria of the water flow and N transport equations. Extremely small time steps were used at the early stages of infiltration. This was relaxed considerably (time steps up to 2 hrs were used) at later stages of water redistribution.

Another restriction is the root uptake of water and nitrogen. The macroscopic approach, even through it provides good predictions, does not include the physiological and physical processes of root uptake. Furthermore, root death, senescence and proliferation were not considered in the model. Further simplification of the model, once the system reaches a

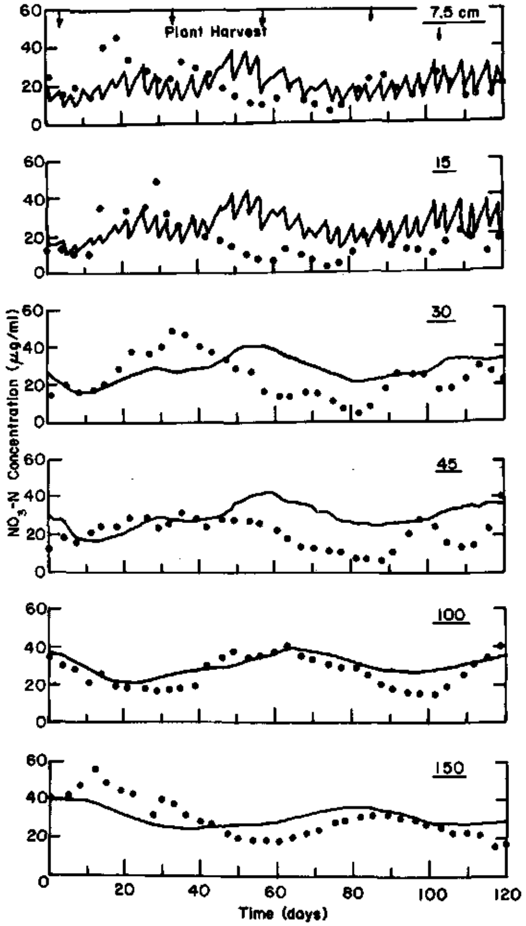


Fig. 4. Comparison between predicted and measured values of NO_3^--N concentrations in soil solutions at different depths in Windsor sandy loam soil (Iskandar and Selim, 1981).

quasi-steady state, is possible but must be verified with experimental data.

13. COMPUTER

The model was developed using an IBM (370/3033) computer system and was adapted to operate on a Prime (480) computer system. At the present time it is operational on both systems.

14. PROGRAM LANGUAGE

The language used is FORTRAN.

15. RUNNING TIME/COST

Approximately 12 minutes of CPU time for 120 days of simulation at a cost of $240.00, IBM 370 with 3033 word processing at L.S.U. was used.

16. USERS

H.M. Selim, I.K. Iskandar and M. Mehran.

17. DEVELOPERS AND PRINCIPAL CONTACTS

Developer of the model: Dr. H.M. Selim.

Dr. H.M. Selim
Agronomy Department
Louisiana State University
Baton Rouge, LA 70803
USA

Dr. I.K. Iskandar
US Army Cold Regions Research and Engineering Laboratory
Hanover, NH 03766
USA

REFERENCES

Claassen, N., and S.A. Barber, 1974. A method for evaluating the influence of concentration on the uptake rate of nutrients. Plant Physiology 54: 564-568.

Davidson, J.M., P.S.C. Rao, and H.M. Selim, 1977. Simulation of nitrogen movement, transformations and plant uptake in the root zone. Proc., National Conference on Irrigation Return Flow Quality Management, Ft. Collins, CO, p. 9-18.

Hagin, J., and A. Amberger, 1974. Contribution of fertilizers and manures to the N- and P-load of waters. A computer simulation, Final Report to the Deutsche Forschungs Gemeinschaft from Technion, Israel.

Iskandar, I.K., and Y. Nakano, 1978. Soil lysimeters for validation models of wastewater renovation by land application - construction, operation and performance. CRREL SR 78-12, USACRREL, Hanover, NH.

Iskandar, I.K., R.S. Sletten, D.C. Leggett, and T.F. Jenkins, 1976. Wastewater renovation by a prototype slow infiltration land treatment system. CRREL Report 76-19, US Army Cold Regions Research and Engineering Laboratory, Hanover, NH 03755.

Iskandar, I.K., S.T. Quarry, R. Bates, and J. Ingersoll, 1979. Documentation of soil characteristics and climatology during five years of wastewater application to CRREL test cells. CRREL Special Report 79-23.

Iskandar, I.K., and H.M. Selim, 1981. Comparison between experimental and simulated nitrogen behavior for slow infiltration systems. In: I.K. Iskandar (ed.) Modeling Wastewater Renovation by Land Application, John Wiley Pub., NY, N.Y.

Jacobson, S., and M. Alexander, 1978. Preliminary investigations of the kinetics of nitrogen transformation and nitrosamine formation in land treatment of wastewater. CRREL SR 79-4.

McLaren, A.D., 1970. Temporal and vectorial reactions of nitrogen in soil. Canadian Journal of Soil Science, 50: 97-109.

McLaren, A.D., 1971. Kinetics of nitrifications in soils. Growth of nitrifiers. Soil Science Society of America Proceedings 35: 91-95.

Mehran, M., and K.K. Tanji, 1974. Computer modeling of nitrogen transformations in soils. Journal Environmental Quality, 3: 391-396.

Misra, C., D.R. Nielsen, and J.W. Biggar, 1974. Nitrogen transformations in soil during leaching: I. Theoretical considerations. Soil Science Society of America Proceedings, 38: 289-293.

Molz, F.J., and I. Remson, 1970. Extraction term models of soil moisture use by transpiring plants. Water Resources Research, 6: 1346-1356.

Nye, P.H., and F.H.C. Marriott, 1969. A theoretical study of the distribution of substances around roots resulting from simultaneous diffusion and mass flow. Plant and Soil, 30: 459-472.

Nye, P.H., and P.B. Tinker, 1977. Solute movement in the soil root system, University of California Press, Berkeley, CA.

Palazzo, A., H.L. McKim, 1978. The growth and nutrient uptake of forage grasses when receiving various application rates of wastewater. Proceedings International Symposium on State of Knowledge in Land Treatment of Wastewater, USACRREL, Hanover, NY, USA, 20-25 August, 1978, p. 157-164.

Selim, H.M., 1978. Transport of reactive solute during transient, unsaturated flow in multi-layered soils. Soil Science, 126: 127-135.

Selim, H.M., J.M. Davidson, P.S.C. Rao, and D.A. Graetz, 1976. Nitrogen transformations and transport during transient unsaturated water flow in soils, Agronomy Abstracts, American Society of Agronomy, p. 123.

Selim, H.M., and I.K. Iskandar, 1978. A simplified nitrogen model for land treatment of wastewater. In International Symposium on Land Treatment of Wastewater, Hanover, NH, p. 171-179.

4.5 Nitrogen dynamics in soil[1]

G. Kruh and E. Segall

1. NAME OF MODEL

Nitrogen dynamics in soil (NDS).

2. SYSTEM MODEL

A two-metre-deep profile of a flat field. The system includes the processes plant uptake, water, oxygen, heat and nitrate movement, and mineralization, nitrification and denitrification of nitrogen.

3. OBJECTIVES

The model calculates nitrogen leaching below depths of two metres from soil surface. Simulating the behaviour of nitrogen under different possible fertilizer treatments, is possible to estimate the nitrogen fertilizer requirements for various soil and climatic conditions.

4. TIME SCALE

The model has been used for up to 200 days. A unsophisticated numerical integration method gives a time resolution of 0.002 days.

5. DIAGRAMS

Figure 1. Ammonification of organic nitrogen and oxydation of ammonia.
Figure 2. Oxygen movement.
Figure 3. Nitrate movement and denitrification.

6. LEVELS

The equations representing different processes are integrated simultaneously. The times of relaxation of the processes included are very different. The mineralization of nitrogen is slow relative to oxygen movement or denitrification.

The following integrals are considered in the model:

- water flow at 1 metre depth
- water content at every layer

---

[1] This presentation is based on work reported in Hagin & Amberger (1974), Kruh (1974) and Kruh (1978).

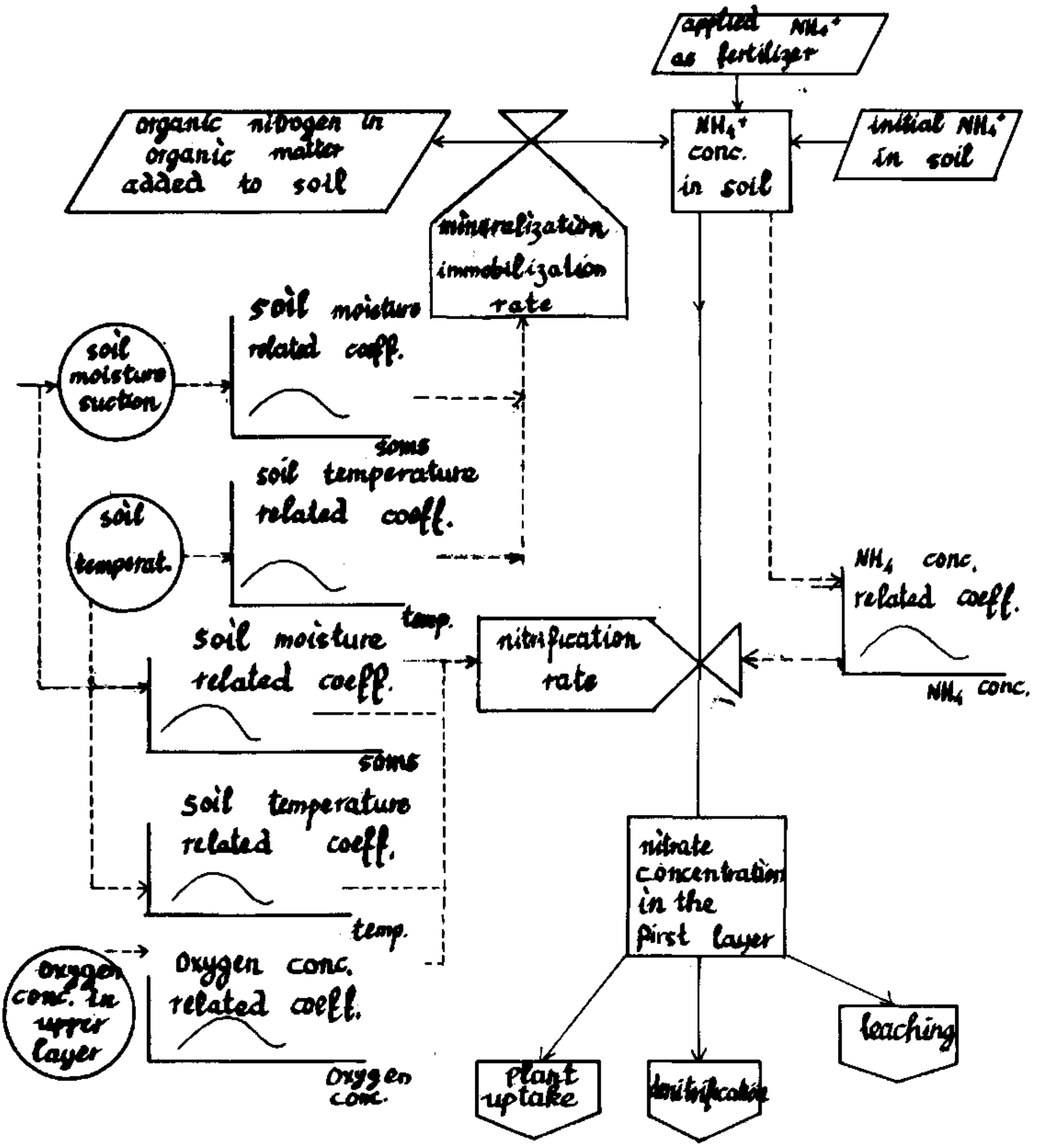
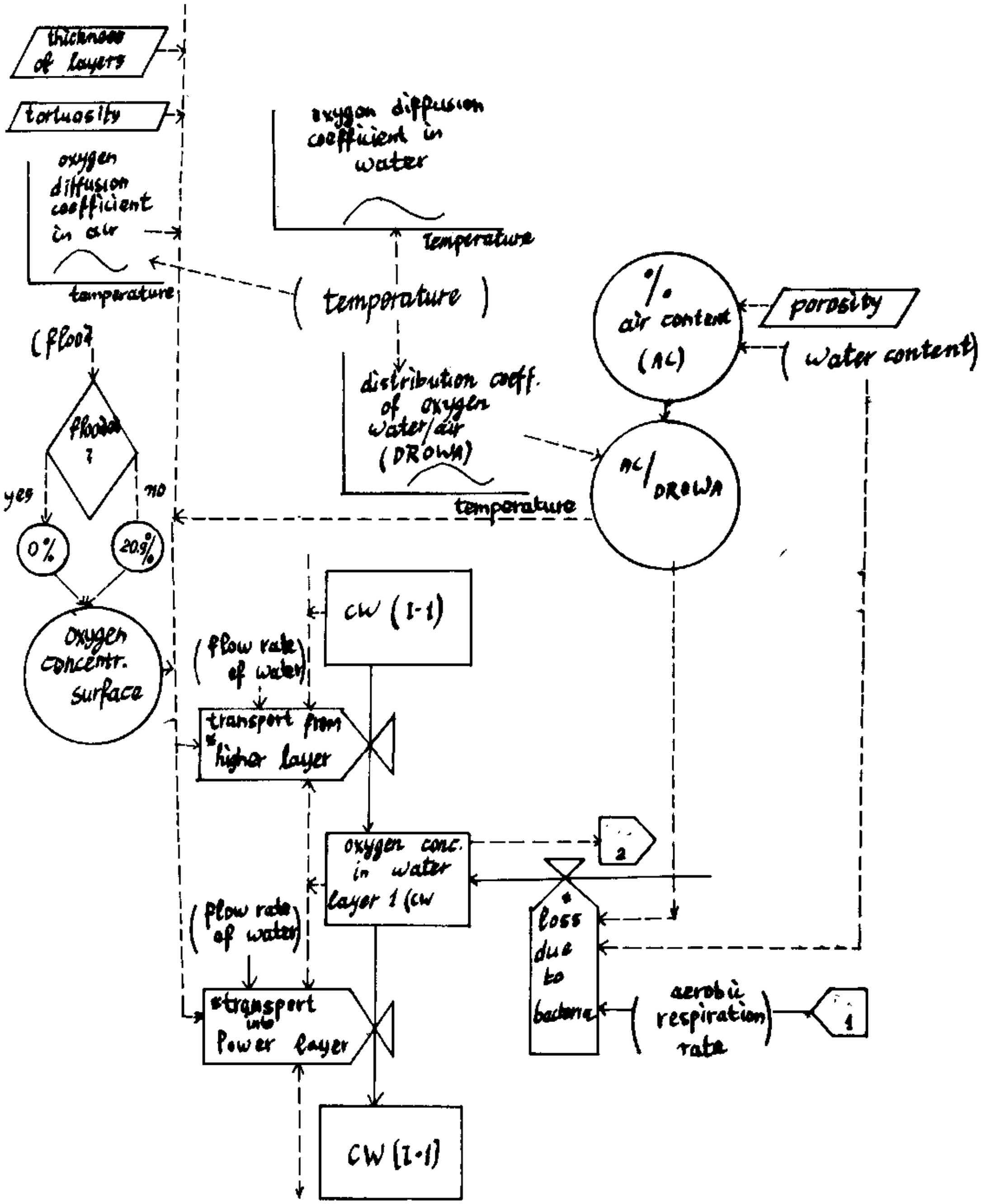


Fig. 1. Ammonification and nitrification of ammonium.



* in the program, these rates are combined into one expression

Fig. 2a. Oxygen movement.

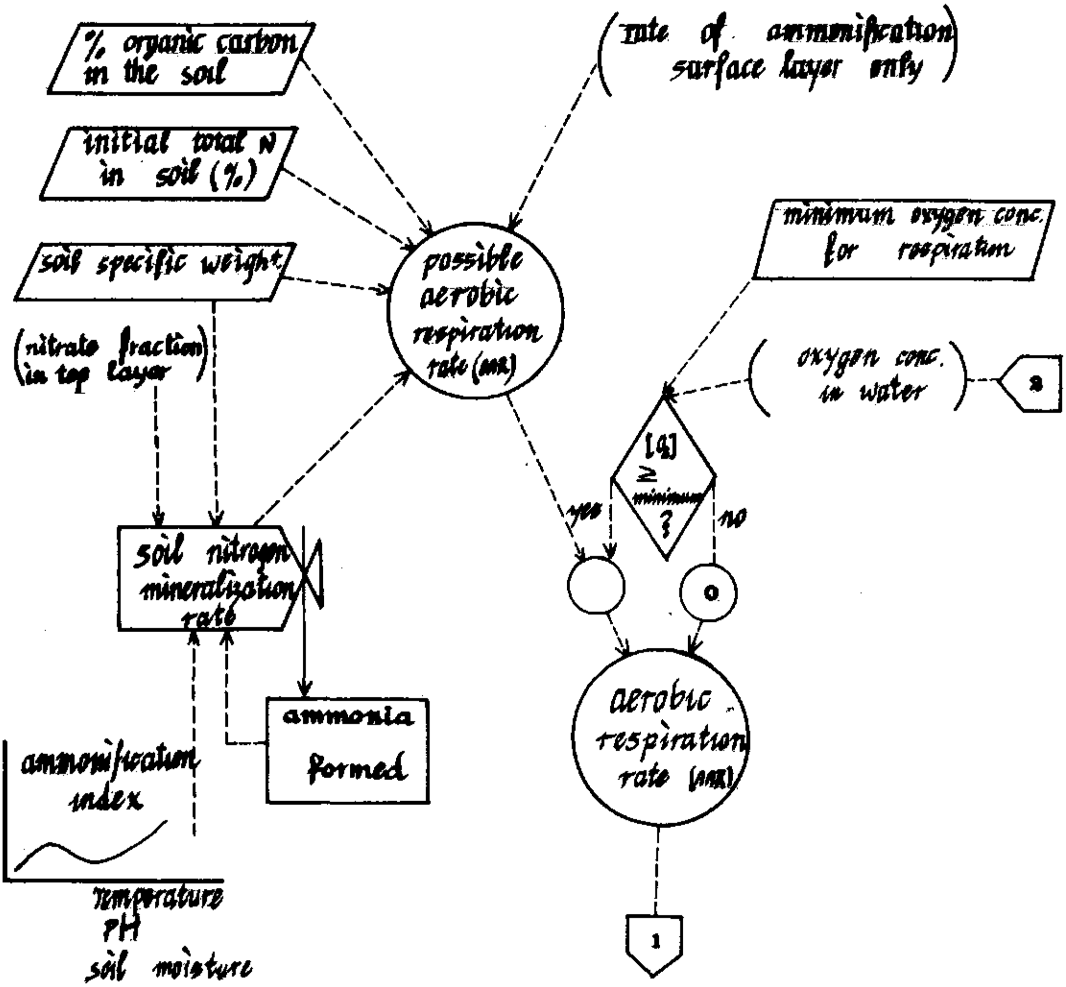
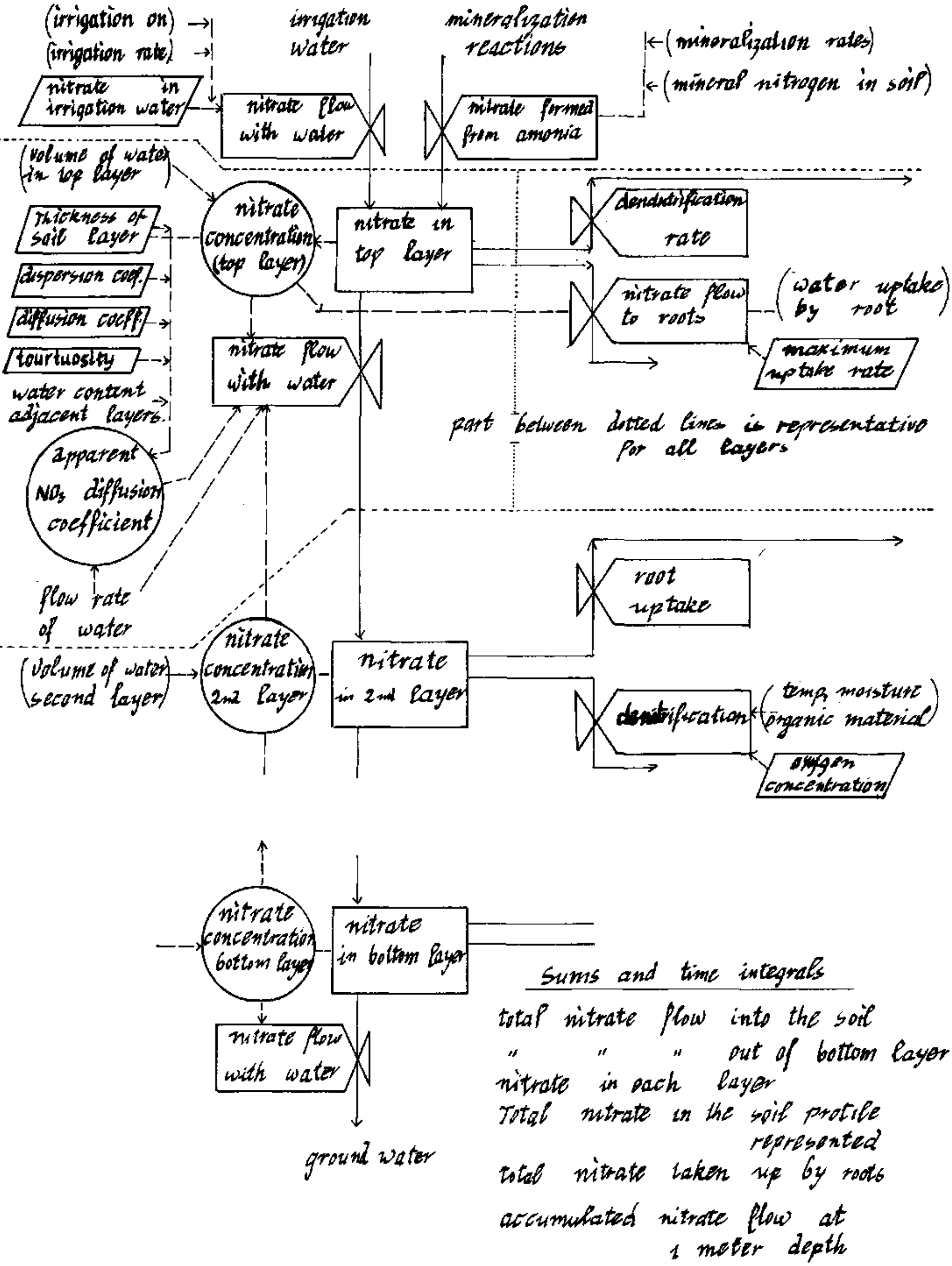

% organic carbon in the soil
rate of ammonification surface layer only
initial total N in soil (%)
soil specific weight
possible aerobic respiration rate (ARR)
minimum oxygen conc. for respiration
nitrate fraction in top layer
oxygen conc. in water
2
$[O_2]$ ≥ minimum ?
yes
no
0
soil nitrogen mineralization rate
ammonia formed
aerobic respiration rate (ARR)
ammonification index
temperature
PH
soil moisture
1

Fig. 2b.



Sums and time integrals

total nitrate flow into the soil
" " " out of bottom layer
nitrate in each layer
Total nitrate in the soil profile represented
total nitrate taken up by roots
accumulated nitrate flow at 1 meter depth

Fig. 3. Nitrate flow.

- water inflow into the top layer of the soil
- water outflow from two metre profile
- water head on soil under flooding conditions
- heat content of each soil layer
- nitrogen immobilized by lignin from organic materials
- nitrogen immobilized by hemicellulose from organic materials
- nitrogen immobilized by cellulose from organic materials
- nitrogen immobilized by sugars from organic materials
- N ammonification of components linked to lignin
- N ammonification of components linked to sugars
- N ammonification of components linked to hemicellulose
- N ammonification of components linked to cellulose
- nitrogen mineralized from humus
- ammonium present in the soil at all times
- nitrates formed during nitrification
- oxygen concentration in soil water
- nitrogen loss by denitrification
- nitrates leached below a depth of one metre
- nitrate concentration in soil
- nitrate leached below a depth of two metres
- nitrate uptake by plants.

7. GOVERNING EQUATIONS

a. *Mineralization of organic nitrogen from soil, humus and manures, and nitrification of ammonia*

From laboratory work, the concentration of nitrate due to mineralization $(NO_3^-)_M$ in soil treated with manure or without any treatment may be approximated by a parabolic function of time:

$$(NO_3^-)_M = A_p + B_p t + C_p t^2 \tag{1}$$

The differential form of that equation is

$$\frac{d\,(NO_3^-)_M}{dt} = \sqrt{B_p^2 - 4C_p[A_p - (NO_3^-)_M]} \tag{2}$$

where A_p, B_p and C_p are parameters established experimentally. In fact this mineralization occurs in two stages: production of ammonia, and oxidation of this ammonia to nitrate. As the first step is much slower than the second, Equation (2) reflects the first step and actually represents the rate of production of ammonia:

$$\frac{d\ (NH_4^+)}{dt} = \sqrt{B_p^2 - 4C_p\ [A_p - (NO_3^-)_M]} \qquad (3)$$

Ammonium will be oxidized to nitrate. The production of nitrates (NO_3^-) , as function of time was formulated by Lees and Quastes (1946) in the form of a logarithmic equation:

$$\log \frac{(NO_3^-)_N}{M - (NO_3^-)_N} = K\ (t - t_{\frac{1}{2}}) \qquad (4)$$

Solving for (NO_3^-) and differentiating with respect to time:

$$\frac{d\ (NO_3^-)_N}{dt} = \frac{M.K.\ln\ 10.10^{K(t-t_{\frac{1}{2}})}.[1+10^{K(t-t_{\frac{1}{2}})} - 10^{K(t-t_{\frac{1}{2}})}]}{[1 + 10^{K(t-t_{\frac{1}{2}})}]^2} \qquad (5)$$

Substituting $10^{K(t-t_{\frac{1}{2}})}$ by $(NO_3^-)_N/[M-(NO_3^-)_N]$, Equation (5) is reduced to:

$$\frac{d\ (NO_3^-)_N}{dt} = (\ln\ 10)\ .\ \frac{K}{M}\ (NO_3^-)_N\ [M - (NO_3^-)_N] \qquad (6)$$

where K is constant, M is the asymptotic value of $(NO_3^-)_N$ and $t_{\frac{1}{2}}$ is the time when $(NO_3^-)_N = \frac{M}{2}$.

Experiments showed that the rate ammonium leaves the system differs from the rate of nitrate formation. The disappearance rate is:

$$\frac{d\ (NH_4^+)}{dt} = -\ K_{NH_4} \qquad (7)$$

which represents a zero-degree pseudo-kinetic equation. Therefore the total amount of ammonium is correlated with the (initial) ammonium concentration in the soil (e.g. from fertilizers, from the mineralization and from the nitrification. Then the total amount of ammonium, M, can be calculated from:

$$M_t = M_{init} + \sum_{o}^{t} [(NH^+_{4_{OM}}) - (NH^+_{4_{OM}})_{t-\Delta t}] \qquad (8)$$

where M_{init} is the initial amount of ammonium fertilizers, and $(NH^+_{4_{OM}})_{t-\Delta t}$ is the ammonium which is nitrified.

b. *Denitrification of nitrates in soil*
This process was treated as a first-order reaction

$$-\frac{d\,(NO_3^-)}{dt} = k_D\ (NO_3^-) \tag{9}$$

where k_D is a function of various factors: temperature, pH, soil moisture, oxygen concentration and availability of electron donors in soil (organic matter).

For an abundant supply of available organic carbon the denitrification rate depends entirely upon the nitrate concentration, expresed in Equation (9). In this case, the availability of organic carbon does not influence the reaction. If the supply of available organic carbon is limited, however, the factor is less than 1. To emphasize this the denitrification rate is expressed as function of available carbon in soil:

$$\frac{d\,(NO_3^-)}{dt} = \left[\frac{k'}{1.0714}\right]^{\frac{1}{2}} \cdot [\Sigma k_i\ (C_i)^{\frac{1}{2}}] \cdot (NO_3^-)^{\frac{1}{2}} \tag{10}$$

where

k = the denitrification rate constant for unlimitated available carbon
k_i = the specific decomposition rate constant for the carbon fraction C
C_i = the concentration of carbon component $\underline{i}$.

c. *Oxygen transfer*

Vertical flow of oxygen through soil air may be expressed by Fick's equation. To obtain changes in the amount of oxygen per unit of soil volume the oxygen of soil air has to be multiplied by the volume of airfilled pores per unit soil volume (V_a), and the amount of oxygen dissolving in the soil water per unit time $\partial S/\partial t$ subtracted.

$$V_a \frac{\partial C_a}{\partial t} = D_a V_a \frac{\partial^2 C_a}{\partial Z^2} - \frac{\partial S}{\partial t} \tag{11}$$

where C_a = oxygen concentration in soil air, D_a = diffusion coefficient in soil air, Z = depth and t = time.

Similarly, the equation for the dissolved oxygen in the soil solution is:

$$V_w \frac{\partial C_w}{\partial t} = D_w V_w \frac{\partial^2 C_w}{\partial t} + \frac{\partial S}{\partial t} - RV_w \tag{12}$$

where V_w = volume fraction of soil water, C_w = oxygen concentration in soil water, D_w = diffusion coefficient in soil water, and R = amount of oxygen consumed by oxidation of ammonia and organic carbon per volume of soil water and per unit time (oxygen sink).

Because there is instantaneous equilibrium between water and air oxygen:

$$C_a = K_{aw} \cdot C_w \tag{13}$$

where K_{aw} is the distribution constant of oxygen between air and water.

The quation describing the flux of oxygen in soil water is obtained by substituting Equation (13) into Equation (11), adding Equation (12) and rearranging the terms:

$$\frac{\partial C_w}{\partial t} = \frac{V_w D_w + K_{aw} V_a D_a}{K_{aw} V_a + V_w} \cdot \frac{\partial^2 C_w}{\partial Z^2} - \frac{R V_w}{K_{aw} V_a + V_w} \qquad (14)$$

where R, the oxygen sink is.

$$R = - \frac{\partial O_2}{\partial t} = \left[\frac{\partial C_{soil}}{\partial t} + \frac{\partial C_L}{\partial t} \cdot \frac{\partial C_C}{\partial t} \cdot \frac{\partial C_H}{\partial t} \cdot \frac{\partial C_S}{\partial t}\right] \cdot 0.16 + \frac{d\ (NH_4^+)}{dt} \cdot 0.32 \qquad (15)$$

where C is carbon oxidized from different sources indicated by the subscripts L - lignin; C - cellulose; H - hemicellulose; S - sugars; and C_{soil} - humus.

For each gram of NH_4^+-nitrogen oxidized 0.32 g of oxygen is consumed. For each gram of carbon, only 0.16 g is consumed.

d. *Water, nitrate and heat transport in soil*

This part of the program is based on the work of De Wit and Van Keulen (1972), although additional phenomena have been incorporated.

Water is added by rainfall and irrigation, and lost by leaching, evaporation and uptake. Nitrates added to or formed in the upper soil layer are transported and lost by diffusion and leaching, as well as denitrification. The effect of heat was also included in this program. because the temperature of the upper soil layer strongly influences the rate of nitrogen reaction there.

For deriving the different equations for leaching the soil profile is divided into a number of homogeneous layers of equal thickness.

e. *Water flow through soil*

The calculation of the rate of water flow is based on an extended Darcy equation:

$$-v = D(\theta) \frac{\partial \theta}{\partial x} + k(\theta) \qquad (16)$$

where v = flow rate of water, D = diffusion coefficient, θ = soil moisture, x = distance, and k = hydraulic conductivity of soil.

Water addition by rainfall is simulated as follows:

Information on rain is arranged in the form of numerical triplets, with the first number representing the time (days) when rain began, the second, the intensity (mm/d) and the third, the time (days) when rain at stated intensity ended.

Flow into the soil and possible flood-head formation is considered under the four possible conditions[1]:

- Irrigation off, no rain, no flooding:

The flow is upward, equal to the rate of evaporation. This evaporation is limited by the conductivity and diffusivity of the soil-air interface.

- Irrigation off, no rain, flooded:

The flow is limited by the diffusivity and conductivity of saturated soil, the limiting infiltration rate. The hydraulic head is also diminished by evaporation.

- Irrigation on, and/or rainfall, no flooding:

If the rates of rainfall and irrigation exceed evaporation and the maximum infiltration rate, flooding will occur.

- Irrigation on, and/or rainfall, flooded:

The flow is limited by the maximum infiltration rate into saturated soil.

Transpiration rates are calculated from the relation:

$$\text{Transpiration} = \text{Class A pan evaporation} \times \frac{\text{evapotranspiration}}{\text{class A pan evaporation}} \times \frac{\text{transpiration}}{\text{evapotranspiration}} .$$

The relevant parameters in this equation are changed every ten days to allow for plant growth and seasonal changes.

The rate of water uptake by roots is assumed to be proportional to the transpiration rates and the water content of soil layers and distributed between the layers according to root activity. However, if soil-moisture tension in a certain layer is above 2 MPa no water is taken from it.

The net flow of water is calculated by subtracting the flow rates of water leaving the last layer and water taken up by plants from the overall rate of flow through the soil profile. Finally, the total amounts of water entering the soil at the surface and leaving the last soil layer are calculated by integration.

f. *Nitrate flow and uptake*

Nitrates are assumed to be completely soluble in water flowing through the soil profile. The increase of nitrate in the profile has three sources: inflow with irrigation or rain water, oxidation of ammonia in the first soil layer, and fertilizers. Nitrogen losses occur by three processes: leaching (below a predetermined soil depth), uptake by plants and denitrification.

In each layer, nitrate accumulation rates are computed by considering interlayer migration, root uptake, and denitrification. In the surface layer, nitrate is also added by

---

[1] Runoff is not considered in the four possible conditions.

oxidation of ammonia.

Interlayer migration is assumed to occur by diffusion of the salt through the soil pores filled with water and/or water films and by mass flow. Dispersion of the sald with the mass flow occurs because of the non-uniform flow velocity in pores of varying size.

Diffusion flow is proportional to the diffusion coefficient and the nitrate concentration gradient between adjacent soil layers, and inversely proportional to the spacing of the layer center lines. The diffusion coefficient for the soil water differs from that of pure water (which is equal to one): it must be multiplied by a tortuosity factor and the water content.

The mass flow is proportional to the water flow, the concentration of nitrates in water and a dispersion coefficient, which ranges from 0.7 cm (for coarse sand) to 7 cm, according to the pore-size distribution.

The rate of uptake from a soil layer is assumed to be the product of the amount of water taken up from that layer and the concentration of nitrates in it. However, as concentrations may be rather high, especially in the upper layer, it seemed appropriate to limit the uptake to a maximum concentration.

g. *Heat flow*

The temperature of any soil layer is calculated by dividing its volumetric heat content by its volumetric heat capacity. The volumetric heat content is calculated by integrating the net heat flux in the layer, which is composed of the heat flowing with water from one layer into another, the heat lost with the transpiration current and the heat lost by conduction. The heat flowing with water in the first soil layer is the product of the flow rate of water in the first layer and the temperature of the irrigation water. For the other soil layers, the temperature of the particular layer or that of the layer above it is chosen according to the direction of the water flow. The transpiration loss is calculated in a similar way. Heat flow by conduction from one soil layer into another is calculated from the average heat conductivity of the two adjacent layers, the temperature difference, and their center-line spacing.

For the first soil layer, the air temperature is taken from tabulated data, with suitable periodic changes. The heat conductivity of a soil varies with its moisture content and may be represented as a function of soil water.

The volumetric heat capacity is the product of the heat capacity of soil minerals (= 0.48, that of silicate minerals) and their relative content plus the heat capacity of the water in the same soil volume.

8. INPUT PARAMETERS

a. *Most important initial values*

- Initial water content, cm^3/cm^3
- Water conductivity at soil-air interface, cm/d
- Water diffusivity at soil-air interface, cm^2/d
- Intensity of irrigation in cm/h

- Tortuosity factor, assumed uniform for all layers
- Heat capacity of minerals, $cal.d^{-1}.cm^{-3}$
- Initial heat content of soil layers, cal/cm^2
- Initial temperature of soil layers
- Initial concentration of NH_4^+ added to soil, µg/g
- Initial amounts of dry manure added to soil in tonnes/ha
- Oxygen concentration in soil water limiting respiration
- Carbon fraction in organic matter added to soil
- Carbon fraction in humus
- Initial concentration of oxygen in water
- Cellulose, hemicellulose, sugars and lignin percentage in organic material added to soil
- Initial concentration of nitrate in soil.

b. *Auxiliary values*
- Soil-water conductivity as a function of water content, cm/d
- Soil-water diffusivity as a function of water content, cm^2/d
- Heat conductivity of the soil at various water content, $cal.cm^{-1}.d^{-1}.K^{-1}$
- Asymptotic value of nitrification (M) versus NH_4^+ added rate constant of nitrification versus asymptotic value of nitrification (M), d^{-1}
- Half-time of nitrification versus added NH_4^+
- Rate constant of nitrification versus temperature
- Half-time of nitrification versus temperature
- Rate constant of nitrification versus moisture
- Half-time of nitrification versus moisture
- Rate constant of NH_4^+ oxidation versus added NH_4^+ µg/g
- Rate constant of NH_4^+ oxidation versus temperature
- Rate constant of NH_4^+ oxidation versus moisture
- Ammonification parameters (A_p, B_p, C_p) versus tonnes of added dry manure
- Ammonification parameters (A_p, B_p, C_p) versus temperature
- Ammonification parameters (A_p, B_p, C_p) versus moisture
- Denitrification rate constant versus temperature
- Denitrification rate constant versus moisture
- Distribution of oxygen between air and water as a function of temperature
- Oxygen diffusion constant in air as a function of temperature
- Daily minimum and maximum air temperatures
- Rain: beginning, intensity, and end of each rainfall
- Class A Evaporation
- Roots activities
- Ratio of evaporation to evapotranspiration
- Ratio of evapotranspiration to class A Pan Evaporation

9. OUTPUT: VERIFIABLE VARIABLES

Concentration of NH_4^+ and NO_3^+ in the soil

Soil moisture

Soil temperature

Water and nitrate outflow (if lysimeters are used)

Plant uptake.

10 and 11. OBSERVATIONS AND COMPARISONS

Experiments to verify the model have been conducted at laboratory and field scale.

Laboratory experiment

Results of incubation of a soil at different temperatures, moistures, and nitrogen inputs were compared with results of programs simulating the basic processes.
Some of the results are described in Figures 4 and 5.

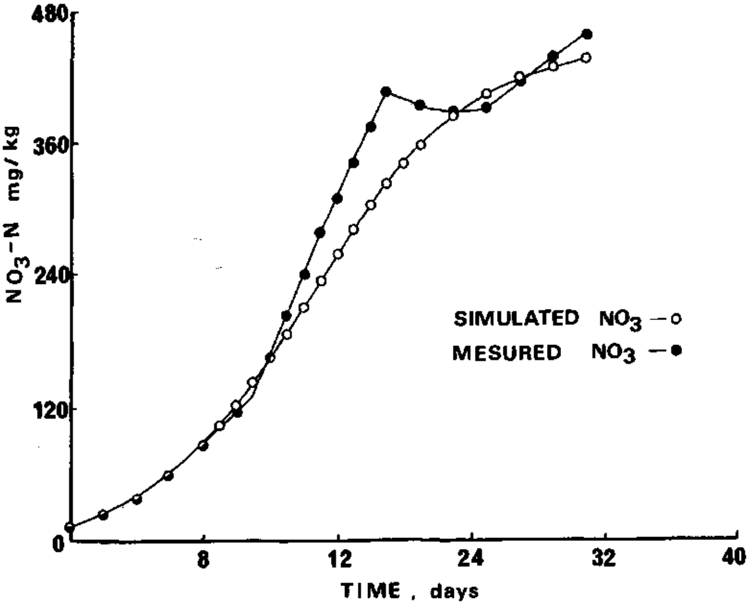


Fig. 4. Comparison of nitrification results in laboratory with simulation results.

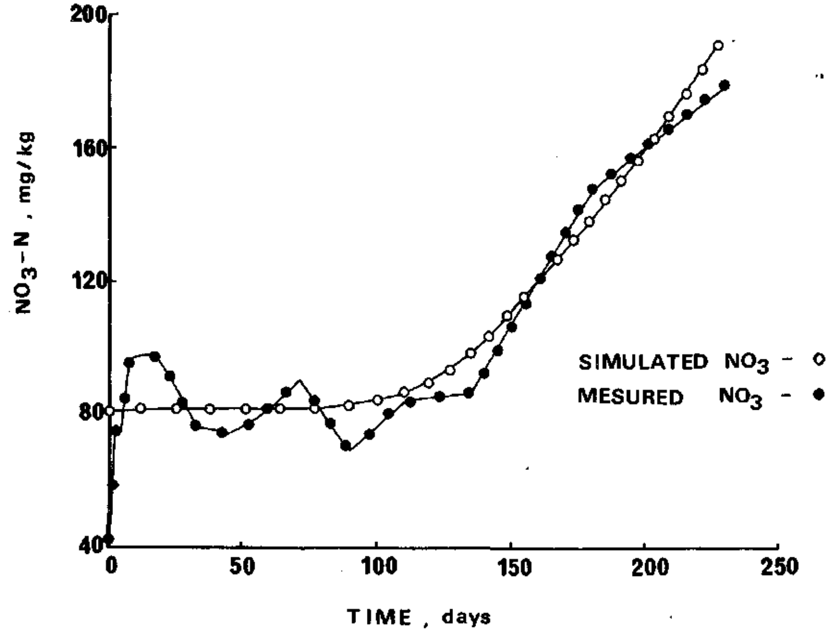


Fig. 5. Comparison of mineralization in laboratory and simulation results.

Field experiment

In a field experiment on cotton, ammonium sulphate was applied in amounts equivalent to nitrogen dressing rates of 60, 120 and 180 kg/ha in winter and early and late spring. A check treatment was included. Soil samples to a depth of 120 cm were taken from time to time, and moisture and nitrate concentrations were measured. For early-spring application, the nitrate distribution in the soil profile showed a maximum in the 20-40 cm depth. The yield could be partly attributed to the nitrate distribution in the soil profile during the early-growth period.

The computer program simulated the nitrate distribution in the soil profile to an accuracy within experimental error. Therefore it was concluded that this program could considerably improve the estimation of nitrogen fertilizer requirements and the optimal timing of applications.

The measured climatic data were used as input for the simulation program. The data included maximum and minimum daily air temperatures, initial soil temperature and rainfall. Soil temperatures were calculated from these data. Some of the input on soil characteristics was taken from experimental data. Input data for hydraulic conductivity, diffusivity, and water retention were taken from measurements on samples of similar soil.

The fertilizer input into the simulation was equivalent to nitrogen dressing rates of

180 kg/ha applied in November. This was in agreement with treatments in the field.

Figure 6 compares measured nitrate concentrations in the field six months after $(NH_4)_2SO_4$ application with those calculated with the simulation program.

The agreement between measured and calculated values indicates the assumptions on reaction kinetics and transport processes in the simulation program reflect field situations reasonably well when allowance is made for sampling variation.

After the program had been calibrated for the 24 November 1975 fertilizer dressings, it was tried out for two other 4 March 1976 (Fig. 7) and 13 April 1976 (Fig. 8).

Most of the simulation results fit the nitrate-concentration curves of field observations.

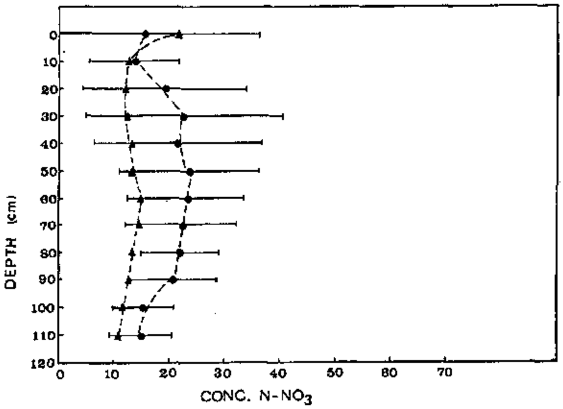


Fig. 6. Comparison of nitrate nitrogen concentrations (mg kg^{-1}) in plots of the field trial treated with 180 kg N as $(NH_4)_2SO_4$ on 24 November 1975 (●) and the simulation results (▲). The sampling date compared is 18 May 1976.

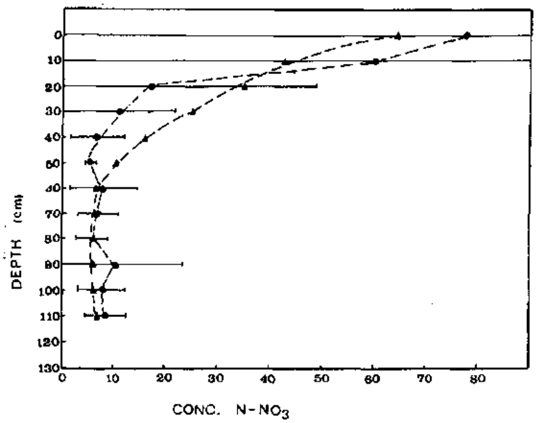


Fig. 7. Comparison of nitrate nitrogen concentration (mg kg^{-1}) in plots of the field trial treated with 180 kg N as $(NH_4)_2SO_4$ on 4 March 1976 (●) and the simulation results (▲). The sampling date compared is 18 May 1976

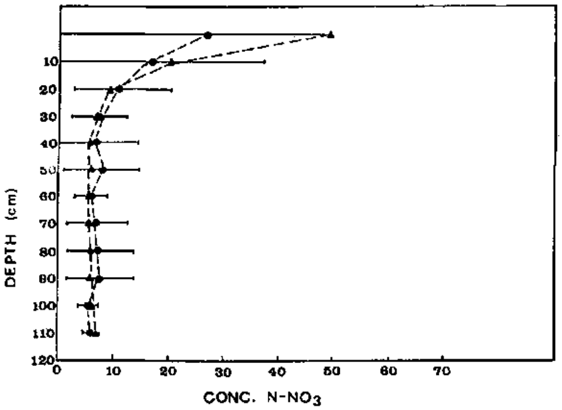


Fig. 8. Comparison of nitrate nitrogen concentration (mg kg^{-1}) in plots of the field trial treated with 180 kg N as $(NH_4)_2SO_4$ on 13 April 1976 (●) and the simulation results (▲). The sampling date compared is 18 May 1976.

12. LIMITS AND LIMITATIONS

Not all the processes included in the program are easy to verify with field data: the extent of denitrification can not be directly measured in a field trial and calculation of root uptake is oversimplified and the results are open to doubt.

Space steps were 10 cm intervals. Time steps, using Euler integration, ranged from 0.02 to 0.0002 days. An improved (CPU-saving) integration method was developed by Amdursky et al. (1980) using FORTRAN instead of CSMP.

13. COMPUTER

IBM 370/68.

14. PROGRAM LANGUAGE

CSMP III.

15. RUNNING TIME

Running the program for two hundred days took 20 minutes of CPU-time.

16. USERS

The model is used at the Soil Science Division of Technion, Haifa, to predict the best time to apply fertilizer to cotton in the northern part of Israel. A calibration of the same program is used at Chapingo, Mexico, by Prof. R. Nunez to predict the movement of nitrates in corn fields. At Göttingen, Federal Republic of Germany, Dr. M. Dianati.

17. DEVELOPER AND PRINCIPAL CONTACTS

The program was developed by J. Hagin and A. Amberger and continued in collaboration with E. Segall and G. Kruh.

The principal contact is Dr. G. Kruh, Soils and Fertilizers Laboratory, Technion-Israel Institute of Technology, Haifa, Israel.

REFERENCES

Amdursky, V., I. Tzur, and A. Ziv, 1980. Some mathematical tools and programming proceedings for soil simulations (see section 5.1 of this publication).

Hagin, J., and A. Amberger, 1974. Contribution of fertilizers and manures to the N- and P-load of waters. Technische Universität München, Institut für Pflanzenernährung and Technion-Israel Institute of Technology, Soils & Fertilizers Laboratory. Final report submitted to the Deutsche Forschungs Gemeinschaft, 124 pp.

Kruh, W.G., 1974. Computer simulation of the contribution of fertilizers and manures to the N- and P-load of waters.(Master's thesis. Abstract computer programs; bibliography tables and figures in English, the rest in Hebrew.) Technion-Israel Institute of Technology, 150 pp.

Kruh, W.G., 1978. Determination of kinetics of nitrogen changes in soil and definitions of parameters of environmental conditions. (Doctoral thesis in Hebrew). Technion-Israel Institute of Technology, 131 pp.

Lees, H., and J.H. Quastel, 1946. Biochemistry of nitrification in soil. I. Kinetics of and effects of poisons on soil nitrification, as studied by a soil perfusion technique. Biochem. J. 40: 803-815.

De Wit, C.T, and H. van Keulen, 1972. Simulation of transport processes in soils. Pudoc, Wageningen, 100 pp.

4.6 Simulation model of the behaviour of N in soil

J.A. van Veen and M.J. Frissel

1. NAME OF MODEL

M_3, this name has not been used in publications.

2. SYSTEMS MODELLED

The model has been developed primarily, for intensive agricultural systems of North-Western Europe. This system is characterized by a temperate climate and high N dressings.

3. OBJECTIVE

The primary objective of this model is to obtain a better understanding of the behaviour of N in agroecosystems and, thus, to optimize fertilizer use. Predictive objectives are secondary. Emphasis is on the role of the micro-organisms. Since carbon is the main limiting substrate in soil controlling the growth and activity of the micro-organisms, this model also aims to describe the impact of the soil C-cycle on the N-transformations.

The model is developed to be generally applicable within the mentioned limitations. Thus the governing equations (see (7)) are site-independent; site-dependent variables such as temperature, moisture content and pH are taken into account with reduction factors. This kind of description allows for study of (a) the validity of hypotheses which are based on data obtained from experiments under controlled conditions in laboratoria and greenhouses, and which are applied for the simulation of N-transformations under field conditions and (b) the combined effect of environmental factors such as temperature and moisture content on several processes of the N-cycle.

4. TIME-SCALE

Simulations have been carried out for periods in the order of months, up to 2 years. When integration methods with a fixed time step were used, this step varied from 0.1 to 0.01 day for the total model and all individual submodels (see (5)) but the denitrification submodel, where a time step of 0.001 day was needed.

5. DIAGRAM

A scheme of the model is shown in Fig. 1. All transformation processes presented in this scheme are described in separate submodels. Submodels are: mineralization and immobilization, nitrification, denitrification, volatilization of ammonia, ammonium fixation on clay minerals and leaching. A detailed scheme of the mineralization and immobilization

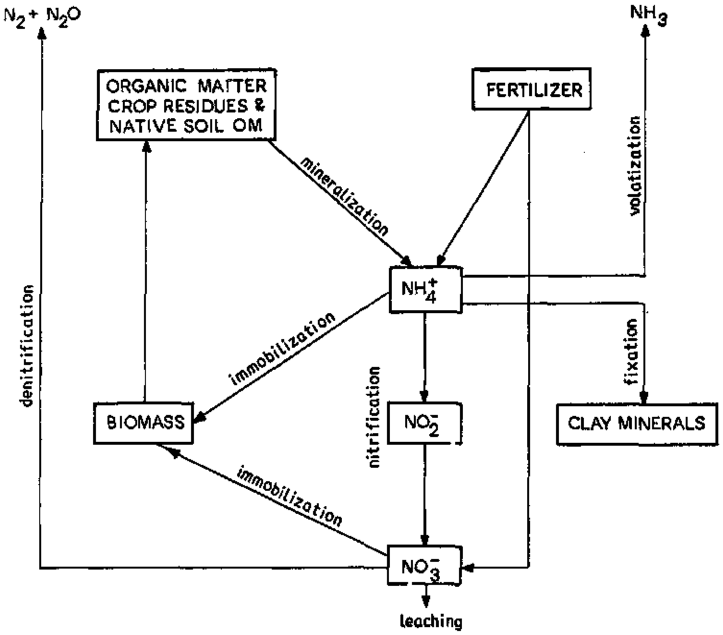


Fig. 1. Scheme of model M_3.

submodel in relation to NO_3^- production and transport is presented in Fig. 2. M_3 is a multi-layer model. The pools or integrals, described in section 6, are identical for all layers. This holds also for all equations (section 7) except in case of the first or upper and last or lower layer, for which adapted in- and output equations are used. The number of layers as well as their thickness, depends on the situation under study. Besides the vertical compartmentalization of the total model, in the submodel of denitrification a radial division of a soil volume around an air-filled pore is considered. In this description the number of layers is fixed (10), their thickness is calculated depending on the relative air volume in the soil (see (7)).

6. LEVELS

The levels or integrals used in the model are:

A. *Nitrogen* (all concentrations in mg $N.g^{-1}$ soil)
A1: Ammonium
A2: Ammonium fixed on clay minerals
A3: Nitrite
A4: Nitrate
A5: Easily decomposable organic-N (pool 3, Fig. 2)
A6: Resistant, active organic-N (pool 5, Fig. 2)

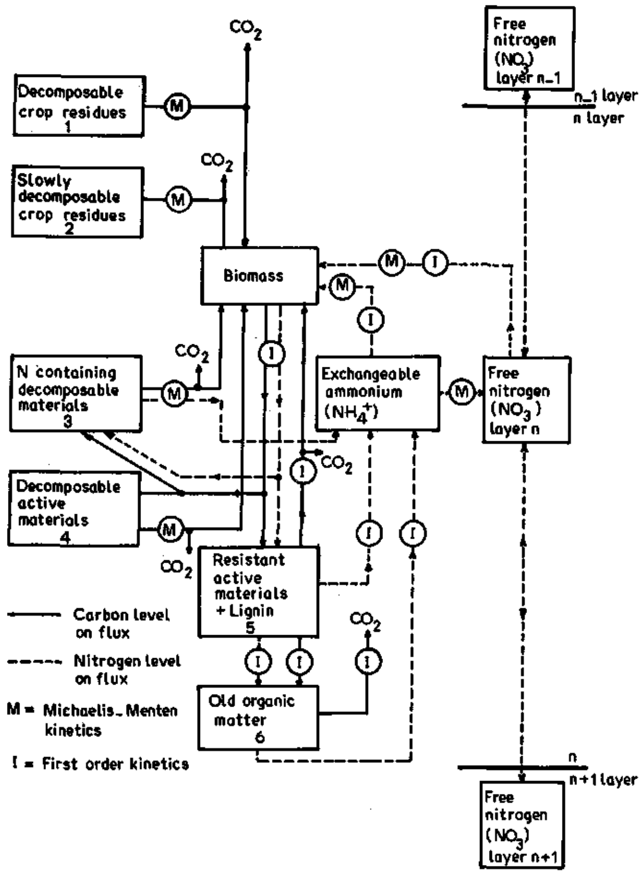


Fig. 2. Scheme of the submodel of mineralization and immobilization in combination with the production and transport of NO_3^-.

A7: Old, recalcitrant organic-N	(pool 6, Fig. 2)

B. *Micro-organisms*

B1: Heterotrophic biomass (mg $C.g^{-1}$ soil)

B2: Ammonium-oxidizing organisms (cells.g^{-1} soil)

B3: Nitrite-oxidizing organisms (cells.g^{-1} soil)

C. *Carbon* (all concentrations in mg $C.g^{-1}$ soil)

C1: Easily decomposable plant residue-C	(pool 1, Fig. 2)
C2: Slowly decomposable plant residue-C	(pool 2, Fig. 2)
C3: Nitrogen containing easily decomposable-C	(pool 3, Fig. 2)
C4: Easily decomposable-C (microbial residues)	(pool 4, Fig. 2)

C5: Resistant active-C (pool 5, Fig. 2)
C6: Recalcitrant, old-C (pool 6, Fig. 2)
C7: CO_2

D. *Other pools*
D1: Oxygen in soil solution (mg $O_2.cm^{-3}$)

Interrelationship between the pools is shown in Figures 1 and 2.

7. GOVERNING EQUATIONS

This section contains a short description of the submodels, which together form the total model. Reduction factors for suboptimal environmental conditions (moisture, temperature) are not shown.

Nitrification

Nitrification is considered to be the result of the activity of two genera of bacteria *Nitrosomonas* which converts NH_4^+ into NO_2^- and *Nitrobacter*, which transforms NO_2^- into NO_3^-. Heterotrophic nitrification is disregarded.

The growth rates of both bacteria, are described with Monod-type kinetics as shown in equation (1).

$$\frac{dA}{dt} = \mu_{max} \cdot \frac{N}{K_n + N} \cdot A - k_A.A \qquad (1)$$

where

A = number of nitrifiers (organisms per unit volume)
μ_{max} = maximum specific growth rate (d^{-1})
N = NH_4^+ or NO_2^- concentration
K_n = saturation constant
k_A = decay rate constant (see section on mineralization and immobilization).

For calculation of the transformation rates of NH_4^+ and NO_2^- due to nitrification (dN/dt), it is assumed that nitrogen is only utilized for energy supply of the nitrifiers (equation (2)), i.e. incorporation of N in the cells is neglected.

$$\frac{dN}{dt} = \frac{1}{Y_N} \cdot \mu_{max} \cdot \frac{N}{K_n + N} \cdot A \qquad (2)$$

where

Y = yield (cells.mg^{-1} N oxidized).

Volatilization of ammonia

Volatilization of ammonia from surface soils is assumed to be controlled by physico-chemical processes. The concentration of NH_3 in the waterphase is calculated from the amount of free and exchangeable NH_4^+ in soil, according to

$$NH_3{}^s + H_2O \overset{K_1}{\rightleftarrows} NH_4^{+s} + OH^- \tag{3}$$

where

NH_4^{+s} = the concentration of NH_4^+ in solution
$NH_3{}^s$ = concentration of NH_3 in solution
K_1 = equilibrium constant.

Then, the equilibrium between the content of NH_3 in the waterphase and NH_3 in the gasphase is calculated (equation (4)).

$$NH_3{}^s \overset{K_2}{\rightleftarrows} NH_3{}^g \tag{4}$$

where

$NH_3{}^g$ = concentration of NH_3 in the gasphase (mg $N.ml^{-1}$)
K_2 = equilibrium constant.

The equilibria (3 and 4) are assumed to be instantaneous, with the equilibrium constants K_1 and K_2 being dependent on temperature.

The dynamic step is the calculation of the amount of gaseous NH_3 which diffuses away from the surface soil into the atmosphere, according to

$$\frac{dN}{dt} = D_{NH_3} \cdot NH_3{}^g/dx_v \tag{5}$$

where

$\frac{dN}{dt}$ = rate of volatilization of ammonia
D_{NH_3} = gas diffusion rate constant ($cm^2 . d^{-1}$)
dx_v = distance between the centre of the top layer and the surface (cm).

To obtain the correct dimensions conversion factors are used which take into account the air-filled volume of soil depending on the moisture content.

Fixation of ammonium on clay minerals

The fixation of ammonium ions on clay minerals is considered to be a purely physicochemical process described by the equilibrium equation:

$$NH_4^+ \text{ (free) } \overset{K}{\rightleftarrows} NH_4^+ \text{ (fixed)} \tag{6}$$

This means that the fixation of ammonium is assumed to be a reversible process between fixed NH_4^+ and free NH_4^+ (exchangeable and soluted NH_4^+). The fixation and release processes are described to be first-order rate reactions. It should be noted, however, that the fixation rate constant is much greater that the constant of release of fixed NH_4^+. Generally, no dynamic equilibrium exists between fixed and free ammonium. The total amount which can be fixed is a preset value.

Mineralization and immobilization

The submodel for immobilization and mineralization has passed three stages during its development. At the first stage the C/N ratio of the organic material was used to control mineralization and immobilization. In a second stage differences in the decomposability of the several compounds of plant residues were concretized and five types of organic compounds were included: (hemi-) cellulose, lignin, sugar, protein and biomass. Carbon-nitrogen ratios of the organic matter were no longer used to control the decomposition, but the uptake of carbon by the growing biomass was determining the decomposition rate. At a third stage the substrate arrangement was revised so that it corresponded better with organic matter distributions as they are used by soil scientists. In this paper only the last version will be dealt with (Fig. 2). For the other two versions the reader is referred to Beek and Frissel (1973), Van Veen (1977) or Frissel and Van Veen (1980).

Mineralization and immobilization are considered to be controlled by the growth and activity of the total microbial biomass in soil. Growth and activity of the biomass is assumed to be limited by the availability of C and N as substrate. To recognize the differences in availability or organic matter-compounds as substrates for micro-organisms both plant residues and soil organic matter are divided into several components.

Crop residue-C is split into sugars and other well decomposable carbohydrates (pool 1) and slowly decomposable material, mostly (hemi-) cellulose (pool 2). The third pool contains all easily decomposable N-containing substances, proteins and amino sugars. The fourth and fifth pool contain microbial debris products and lignins, which thus provide a base for chemical stabilization of organic matter.

Thos fractions can be considered to be the 'active fraction', according to Jannson's (1958) nomenclature. The difference between pool 4 and pool 5 is based on the consideration that material of pool 5 consists of organic matter which is adsorbed on clay minerals or entrapped in soil aggregates, but which is chemically identical to the material in the pool 4 (Paul and Van Veen, 1978). On the contrary, the material of pool 6 is considered to be chemically resistant, i.e. recalcitrant, old organic matter.

As soon as part of the carbon is used for the biomass synthesis, a corresponding quantity of nitrogen (depending on the C/N ratio of the biomass and the substrate) is transferred to the mineral nitrogen pool. The nitrogen flux from the old organic matter to the mineral nitrogen pool is the only one which is not controlled by the soil biomass and biomass growth is not considered with carbon of this pool as substrate. The types of the conversion processes in Figure 2 are indicated with 1 for processes described by first-order rate kinetics and with M for those ones described by Monod-type kinetics.

When using Monod-type kinetics, the reaction rates depend on the amount of biomass which is involved in the utilization of a particular substrate, x. Therefore, it is assumed that each of the carbon pools is utilized by a fraction of the total biomass with the fraction being proportional to the ratios of the amount of the particular carbon compound to the total amount of carbon in pools 1-5.

A typical set of equations for the growth of that part of the biomass which is involved in the decomposition of component x is therefore,

$$dB_x/dt = \mu_x \ . \ B \ . \ C_x/C_T \qquad (7)$$

where

μ_x = relative growth rate of biomass on component x (d^{-1})
B = total microbial biomass (mg $C.g^{-1}$ soil)
C_x = carbon present in component x (mg $C.g^{-1}$ soil)
C_T = total carbon content in pools 1-5 (mg $C.g^{-1}$ soil)

The relative growth rate is calculated by

$$\mu_x = V_{m,x}/(K_m,x + C_x) \ . \ C_x . f(NO_3,NH_4) \qquad (8)$$

where $V_{m,x}$ is the maximum specific growth rate (d^{-1}) and $K_{m,x}$ is the saturation constant (mg $C.g^{-1}$ soil), $f(NO_3,NH_4)$ is a function which sets μ_x to zero if neither NO_3^- nor NH_4^+ is available; if NO_3^- and/or NH_4^+ is available $f(NO_3,NH_4)$ is set to 1.

The decay rate of the biomass depends on the type of biomass. The types which grow on easily available compounds are assumed to have a fast turnover rate, the types which grow on the resistant fractions turnover slowly.

Consequently, the decay of the biomass is described with five equations of the type

$$dB_{D,x}/dt = k_{D,x} \ . \ C_x/C_T \ . \ B \qquad (9)$$

in which $k_{D,x}$ is the specific decay rate constant for the type of biomass which is involved in the decomposition of component x. The specific decay rate constant is linearly related to the 'maintenance coefficient'.

From the difference between dB_x/dt (growth rate biomass) and $dB_{D,x}/dt$ (decay rate biomass) the net growth of biomass component x can be calculated.

To obtain the carbon losses from pools (1-4), it must be taken into account that part of each compound x is used for biosynthesis and the other part for energy production and related CO_2 production. So the utilization rate of C for biosynthesis, dC_x^B/dt, is

$$dC_x^B/dt = dB_x/dt \tag{10}$$

and the CO_2 production equals

$$dCO_{2,x}/dt = dB_x/dt.(1-Y_x)/Y_x \tag{11}$$

where Y_x is the growth yield (mg biomass-C.mg^{-1} substrate-C) and the total utilization rate of C, is found by summation of dC_x^B/dt and $dCO_{2,x}/dt$.

The rate of loss of C from pools 5 and 6 is calculated according to first-order kinetics. So for pool 5 the rate of decomposition dC_5/dt equals

$$dC_5/dt = k_5 \, . \, C_5 \tag{12}$$

where

k_5 = first-order rate constant (d^{-1})
C_5 = content of pools 5 (mg C.g^{-1} soil).

The decomposition of compounds of pool 6 is simulated in the same way. Growth of the biomass on C from pool 5 is calculated by

$$dB_5/dt = Y_5 \, . \, dC_5/dt \tag{13}$$

where Y_5 is the growth yield. The CO_x-production is calculated by

$$dCO_2/dt = (1-Y_5) \, . \, dC_5/dt \tag{14}$$

Finally, the nitrogen mineralization rate is calculated from the decomposition rate of the N-containing components by dividing the carbon transfer rate by the C/N ratio of the components. The immobilization rate is proportional to the growth rate of biomass (expressed in C equivalents) and is thus calculated by dividing the growth rate of the biomass by the C/N ratio of the biomass.

Denitrification

Denitrification is assumed to occur under anaerobic conditions. Therefore, besides the utilization of NO_3^- under anerobic conditions, also the occurrence of these conditions in soil is described. This means, in fact, a description of the behaviour of oxygen. In fully waterlogged soils supply of oxygen is thought to occur by diffusion through water-filled pores from the atmosphere above the soil. Then transport of oxygen through the soil can be described as a function of the concentration gradients (compare the migration of NO_3^- to be discussed later).

In non-waterlogged soils the oxygen supply occurs mainly via air-filled pores. The model considers as rate limiting step the diffusion of oxygen from air-filled pores into the surrounding soil. Based on Henry's Law,

$$P = h_k \cdot X \tag{15}$$

where

X = the molecular fraction of compound, X, in solution

P = partial pressure of X in the gasphase

h_k = constant

the oxygen concentrations in an infinitly thin layer of soil water around an air-filled pore is calculated depending on the partial pressure of O_2 in the soil atmosphere. Diffusion of O_2 in solution through the soil around the pore is calculated based on concentration gradients only (Fig. 3). So,

$$Rd = D_{O_2} \cdot f_t \cdot \theta \cdot [(O_2)_n - (O_2)_{n+1}]/dx_d \tag{16}$$

where

Rd = rate of diffusion of O_2 (mg $O_2 . d^{-1}$)

D_{O_2} = diffusion coefficient of O_2 in solution ($cm^2 . d^{-1}$)

f_t = tortuosity factor. This labyrinth factor depends on the water content, but is less than 1 (Frissel et al., 1970)

θ = water content of the soil around the air-filled pores ($cm^3 . cm^{-3}$)

$(O_2)_n$ = O_2-concentration in layer n (mg $O_2 . cm^{-3}$)

dx_d = diffusion distance (cm)

A similar equation is used for the diffusion of NO_3^- through the soil volume surrounding the air-filled pores.

To calculate the diffusion of oxygen from the air-filled pores to sites where oxygen consumption occurs, the soil around the air-filled pores, which are considered to be cylindrical-shaped, is divided into 10 concentric layers as shown in Fig. 3. The number of pores per unit volume of soil and their thickness depends on the moisture content of the soil and its pF-curve. The mean pore radius at a certain moisture content is calculated according to

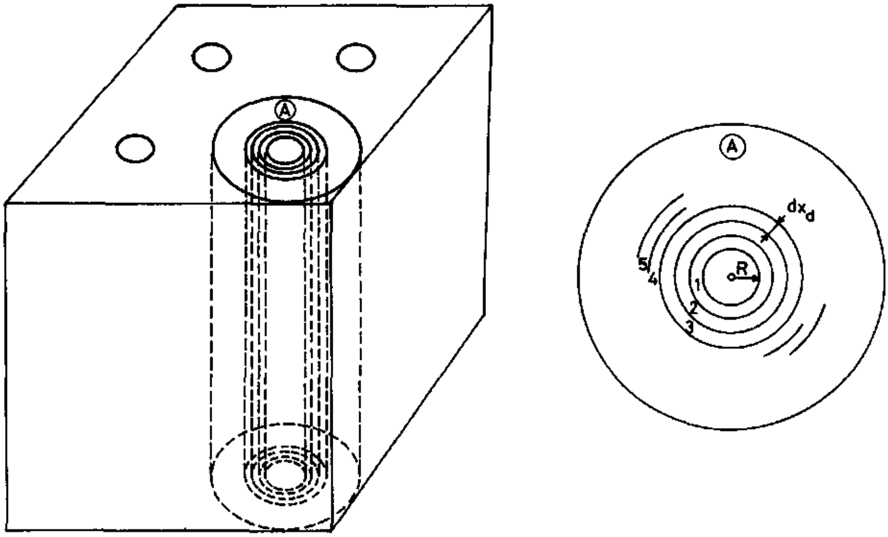


Fig. 3. Schematic picture of the distribution of 4 air-filled pores and the subdividing of the surrounding soil layers, in a soil volume of 1 cm^3.

$$R = 2\sigma/(S_m \cdot 10^3) \tag{17}$$

where

R = pore radius (cm)
σ = surface tension of water (dynes . cm^{-1})
S_m = moisture suction (mbar). S_m can be derived from the pF-curve, pF being defined as the negative logarithm of the moisture suction (cm).

The number, N , of air-filled pores per cm^3 is

$$N_p = V_A/\pi R^2 L \tag{18}$$

where

V_A = total air-filled volume per cm^3 of soil
L = length of the pores = 1 cm.

The thickness of the layers is

$$dx_d = (\sqrt{1/\pi N_p} - R)/10 \tag{19}$$

The consumption rate of $O_2 (dO_2/dt)$ and (in absence of O_2) of NO_3^- (dNO_3^-/dt), is assumed to be proportional to the growth rate of the heterotrophic biomass (dB/dt) which is calculated in the submodel of mineralization and immobilization. So,

$$\frac{dO_2}{dt} = \frac{1}{Y_{O_2}} \cdot \frac{dB}{dt} \tag{20}$$

and

$$\frac{dNO_3^-}{dt} = \frac{1}{Y_{NO_3}} \cdot \frac{dB}{dt} \tag{21}$$

where Y_{O_2} and Y_{NO_3} are the growth yields for O_2 and NO_3^- respectively (mg biomass-C.mg^{-1} O_2 consumed and mg biomass-C.mg^{-1} NO_3 consumed, respectively).

Leaching

It is assumed that nitrate is the only nitrogen component which migrates, thus, transport of NH_4^+ is not considered. The simplified transport equation is:

$$dN_L/dt = D_A \cdot (N_n - N_{n+1})/dx + L_e . F_L . (N_n + N_{n+1})/2$$

where

dN_L/dt = amount which passes the boundary between the layers n and n+1
D_A = apparent diffusion coefficient
N_n = concentration of NO_3^- in compartment n
dx = distance between centres of compartments n and n+1
F_L = moisture flux
L_e = leaching efficiency factor

and

$$D_A = \theta \cdot F_L \cdot D_{NO_3} + d \cdot f_t \tag{23}$$

where

θ = moisture content
f_t = tortuosity factor
D_{NO_3} = diffusion coefficient in water
d = dispersion distance.

8. INPUT PARAMETERS

a. *Initial values of integrals*

The input parameters M_3 needs are:

1. Initial contents of the pools containing N as mentioned in section 6 under A (1-7).
2. Initial contents of the pools containing C as mentioned in section 6 under C (1-6).

The initial amount of CO_2 produced is always zero.

3. Initial number of nitrifying organisms as mentioned in section 6.
4. Initial biomass (mg $C.g^{-1}$ soil).
5. Initial O_2 concentration in the soil atmosphere (mg $O_2.\ cm^{-3}$).

b. *Biological constants*

1. Michaelis-Menten constants, i.e. maximum specific growth rate (d^{-1}) and saturation constant (mg C or $N.g^{-1}$ soil), of nitrifying organisms and micro-organisms involved in the decomposition of organic matter components of pools 1-4 (Fig. 2).
2. Growth yields or efficiency factors to calculate the production of cellular material from the amount of substrate which is utilized. For the nitrifying organisms growth yields are in $cells.mg^{-1}$ N oxidized and for the organisms involved in the decomposition of organic matter of pool 1-5 (Fig. 2) in mg $C.mg^{-1}$ biomass.
3. Decay rate constants of the heterotrophic biomass and nitrifying organisms (d^{-1}).
4. Decomposition rate constant of organic matter of pool 5 and 6 (Fig. 2) (d^{-1}).

c. *Other constants*

1. Equilibrium constants of the reactions presented as equation (3), (4) and (6).
2. Diffusion coefficients ($cm^2.d^{-1}$) of gaseous NH_3 (equation (5)), O_2 and NO_3^- in water (equations (16) and (23)).
3. Tortuosity factor (equations (16) and (23)).
4. Henry's Law constant (equation (15)).
5. Surface tension of water ($dynes.cm^{-1}$) (equation (17)).
6. Leaching efficiency factor (equation (22)).

d. *Other parameters not mentioned in the equations of section 7*

1. Bulk density of the soil ($g.cm^{-3}$).
2. Cation exchange capacity (mg $N.g^{-1}$ soil).
3. pH.
4. Maximum fixation capacity of the soil (mg $N.g^{-1}$ soil).
5. C/N ratios of the proteins, biomass and pools 3, 5 and 6 (Fig. 2).
6. Coefficient to fractionate microbial residues in decomposable and recalcitrant components which are 'protected' and 'non-protected' in soil (Paul and Van Veen, 1978).

e. *Input variables, independent on time*

1. Functions to describe the effect of moisture and temperature on the activity of

of nitrifying organisms.

2. Functions to describe the effect of moisture, temperature (Fig. 4) and oxygen concentration on the activity of the heterotrophic biomass.
3. Moisture retention curve (equation (17)).
4. Layer thickness (cm).

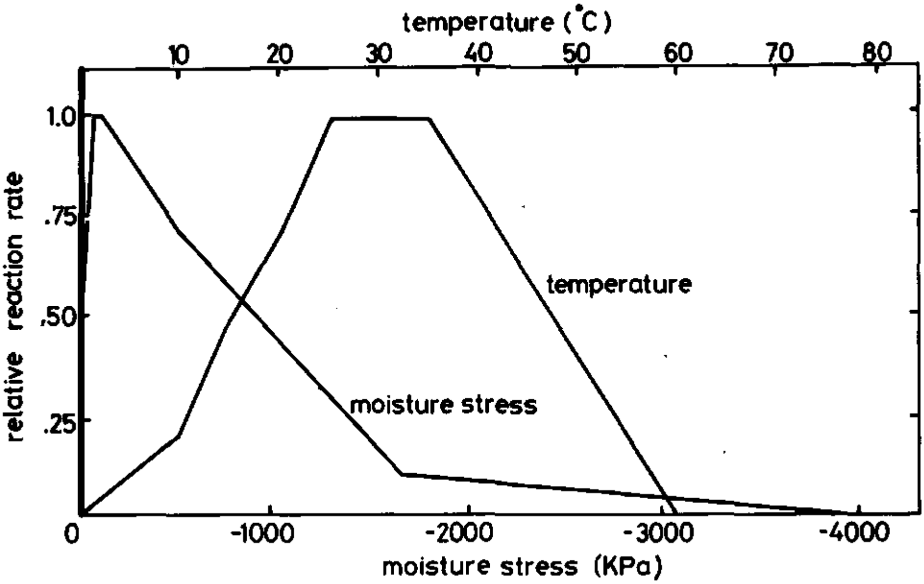


Fig. 4. Reduction factors for the effect of temperature and moisture on the decomposition rate of soil organic matter.

f. *Input parameters varying with time*

1. Temperature (°C).
2. Moisture content ($cm^3.cm^{-3}$).
3. Addition rate of plant residues.

9. OUTPUT, VERIFIABLE VARIABLES

The potentially verifiable output variables are the values of the integrals listed in section 6. Although there are several fractionation techniques of soil organic matter, a precise measurement of the quantity of the organic matter components as indicated by pool 3-6 in Fig. 2, is very questionable. Thus, the main output variables, which are accessible for experimental verification, are:

a. Inorganic nitrogen, NH_4^+ (exchangeable and fixed), NO_3^-, NO_2^-.
b. CO_2^-, O_2.

c. Total microbial biomass.
d. Nitrifying organisms.
e. Crop residue components.

10. OBSERVATIONS

The experiments described here as well as most of the comparison results (section 11) and the equations (section 7), have already been published elsewhere or are in press (Van Veen, 1977; Frissel and Van Veen, 1978; Frissel and Van Veen, 1980 and Van Veen et al., 1980).

The separate submodels were mainly tested on the base of data of experiments described in literature (Van Veen, 1977). Besides those tests of the submodels, two experiments have been carried out to test the total model.

Experiment 1 which was carried out in cooperation with the Institute for Soil Fertility, Haren, was a combined greenhouse/field experiment.

In the pot experiment 8 g of barley straw and 7.5 mg of $(NH_4)_2SO_4$-N was applied per kg soil (fraction of soil > 50 μm 95%, organic C-content 1.23%, organic N-content 0.06%, pH (KCl) 4.6). The soil was kept free from vegetation. During the experiment the temperature ranged from 20-26 °C and the moisutre content was kept at about 60% of the waterholding capacity. The biomass, with the direct microscopy technique, the total N-content, NO_3^- and NH_4^+ were measured at regular intervals.

Similar treatments were used in the field experiment. This experiment was carried out in the same soil as was used for the pot experiment. Inorganic N-content, biomass and Cl^-, to measure transport, were measured every fortnight. Rainfall and groundwater level were measured daily and the temperature of the atmosphere immediately above the soil surface was determined continuously.

Another field test, experiment 2, was done on the base of data from experiments of the IJsselmeerpolders Development Authority, at Lelystad. Those experiments were carried out from November 1975 to February 1977 at a recently reclaimed soil in the IJsselmeerpolders. The soil was rich in soil organic matter. Before the observations started the area was used for flax with the stubbles of flax being ploughed in. Each week the soil was sampled (5 layers of 20 cm each), the samples were analysed for soluble nitrate and incidentally for ammonium which was usually only present as trace. Therefore ammonium and nitrate were determined together as mineral nitrogen. The most important additional observations were temperature, soil moisture and rainfall. During the observation period the soil was kept fallow.

11. COMPARISON RESULTS

For simulating the experiments 1 and 2 as described in section 10 M_3 consisted of all submodels but the denitrification submodel. This could not yet be included because of programming problems, which mainly dealt with the combination of descriptions on vertical transport as used to simulate leaching, and radial or horizontal movement as used to simulate O_2 diffusion.

When using the second version of the submodel of mineralization and immobilization, in which only plant residue-C was considered to be available as substrate for micro-organisms rather serious disagreements between experiment and model occurred as shown in Fig. 5 for inorganic nitrogen. Similar disagreements were found when comparing the experimentally determined and simulated biomass vs time. An inadequate description of the availability of native soil organic matter, including microbial residues, as substrate for micro-organisms was the main reason for those disagreements. Based on these observations the third version of the mineralization and immobilization submodel was developed, which is described in section 7.

When including this version of the submodel in M_3 a much better fit was obtained as shown for the inorganic nitrogen behaviour in the NS-treatment of the greenhouse experiment in Fig. 5. Further testing of M_3 with data from fallow, recently reclaimed soils of the Lake IJssel-polders (experiment 2, see section 10), showed a satisfactory fit (Fig. 6) but imperfections still remain.

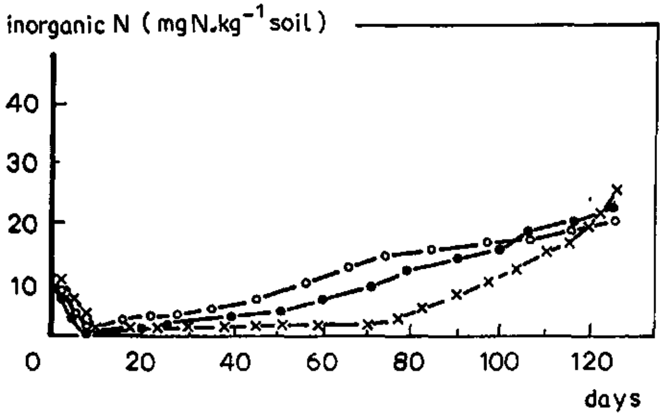


Fig. 5. Comparison of simulated and experimentally determined inorganic-N concentrations in soil vs time after application of straw and N (greenhouse experiment 1).
o–o experiment.
x–x simulation with second version of the model.
o–o simulation with third version of the model.

Verification of separate submodels has mainly be done based on data from literature. Excellent fits were obtained for nitrification in aquatic systems as shown in Fig. 7. However, when using growth rates of nitrifying organisms as determined in soil, a very delayed pattern of NH_4^+ and NO_3^- oxydation is obtained, which does not agree with experimental results found in literature. Including the submodel of nitrification in this way in M_3

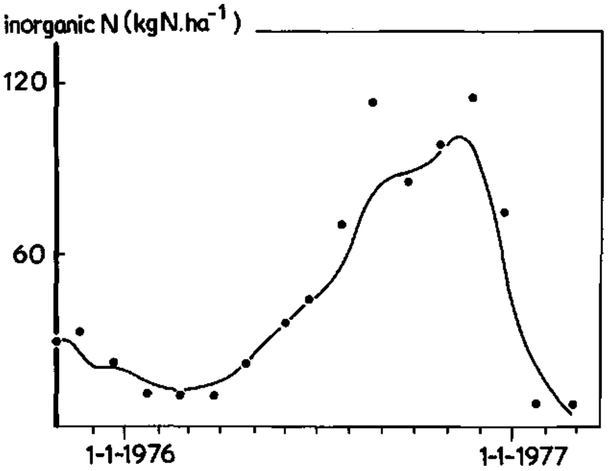


Fig. 6. Calculated (line) and observed (dots, see Figure 10). Inorganic nitrogen of the top 20 cm in function of time as determined in experiment 2.

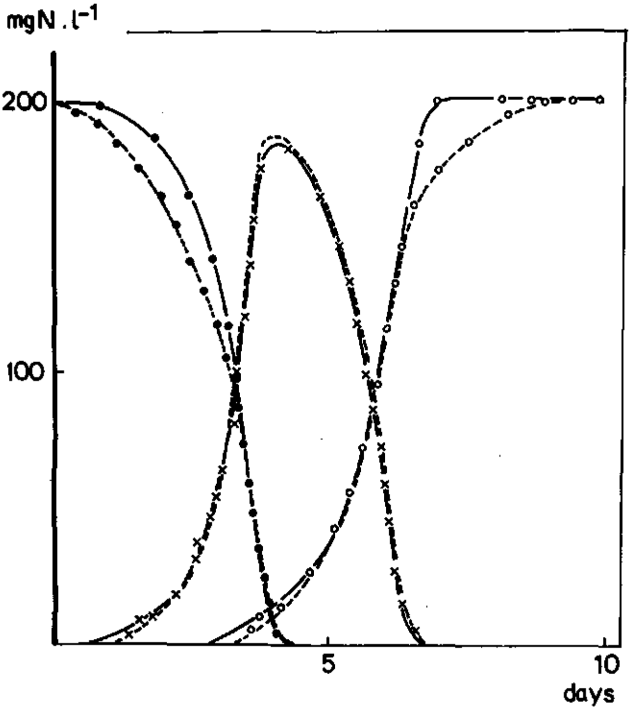


Fig. 7. Comparison of experimental and simulated data on nitrification in aquatic systems. Solid line: simulation; dotted line: experiment. •-• NH_4^+; x-x NO_3^-; o-o NO_3^-.

leaded to inacceptable discrepancies with experimental results. To our opinion, this bad fit is mainly caused by errors in the determination of the values of the specific growth rates of nitrifying organisms in soil.

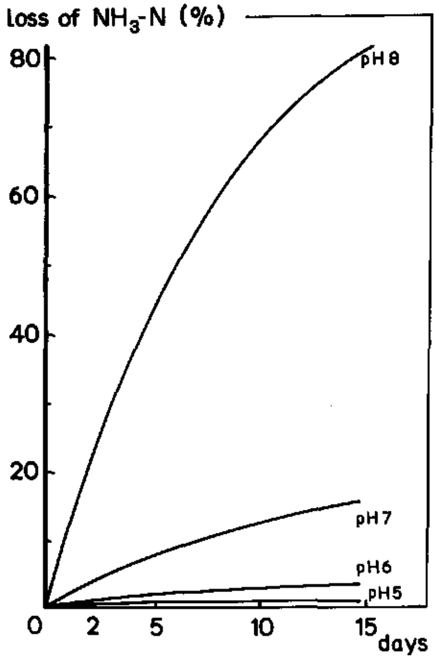


Fig. 8. Calculated loss of ammonia at different pH due to volatilization.

Figure 8 shows the computed effect of pH on the loss of surface applied nitrogen due to ammonia volatilization. These results agree satisfactory with data of Mills et al. (1974) who found up to 17% loss of NH_3-N at pH 7.2 but 63% at pH 8.0-8.5 during a period of 7 days.

Similar comparisons with data from literature are hardly possible for the submodels of ammonium fixation and denitrification, because of lack of data suitable for comparison (Van Veen et al., 1980).

The submodels of mineralization and immobilization and leaching have also been compared separately with data from literature (Van Veen, 1977). However, for a judgement it is more appropriate to consider the comparison between calculations and experiments mentioned in section 10.

Further development of the model will include more experimental verification, including plant growth and with respect to modelling aspects, the development of submodels of the effect of plants on the soil N-transformations and of N_2-fixation, while also priority will be given to combine the submodel of denitrification with the other submodels. Moreover, laboratory and field experiments will be carried out to obtain more insight in the value of data from laboratory experiments on microbial growth and to obtain appropriate data on microbial turnover, which appears a major parameter in this model and, generally, in the role of micro-organisms in nutrient cycles in soil.

12. LIMITS AND LIMITATIONS

There are no particular limitations to the model except the problems on combining descriptions on vertical and horizontal transport processes as already mentioned in section 11.

13. COMPUTER

Use is made of the DEC-10 computer system of the Agricultural University, Wageningen. The program is operational under the TOPS-10 operation system.

14. PROGRAM LANGUAGE

The language used is CSMP3, i.e. Computer Simulation Modelling Program version 3.

15. RUNNING TIME/COST

The computing time for the separate submodels is less than 1 min. for a simulated period of up to 100 days, except in case of the submodel for denitrification with a computing time of approximately 1.7 min. for 3 days. To simulate experiment 1 for 200 days, the computing time of M_3 was approximately 6 min. The computing time of the program used to simulate experiment 2 was approximately 2 min.

Although the simulated period was longer in the latter case (up to 480 days) the difference in computing time is mainly caused by a smaller time step used in the former case, 0.01 day vs 0.1 day, and more compartments 13 vs 5.

One minute CPU time costs approximately 15 Dutch guilders = $7.50.

16. USERS

The model has been used in a variety of studies. Besides the ones mentioned in sections 10 and 11, it was used for studies on soil nitrogen transformations in arid areas, such as Mali and the Sahel and in Canada and other European countries besides The Netherlands.

17. DEVELOPER AND PRINCIPAL CONTACTS

The authors of this paper are also the developers of the model.

ACKNOWLEDGEMENTS

The authors wish to express their gratitude to Ir. G.J. Kolenbrander of the Institute for Soil Fertility and Mr. A.M. Smook of the IJsselmeerpolders Development Authority for their contribution in the verification of the model.

REFERENCES

Beek, J., and M.J. Frissel, 1973. Simulation of nitrogen behaviour in soils. Wageningen: Pudoc, 67 pp.

Frissel, M.J., P. Poelstra, and P. Reiniger, 1970. Chromatographic transport through soils. Plant and Soil 33: 161-176.

Frissel, M.J., and J.A. van Veen, 1978. Critique of computer simulation modelling for nitrogen in irrigated croplands. In: Nielsen, D.R. & McDonald, J.G. (Eds.). Nitrogen in the environment: Vol. 1. Nitrogen behaviour in field soils, pp. 145-162. New York - San Francisco - London: Academic Press.

Frissel, M.J., and J.A. van Veen, 1980. Validation of a simulation model for nitrogen immobilization and mineralization. In: Iskandar, I.G. (Ed.). Simulating nutrient transformation and transport during land treatment of wastewater. Chapter 9 (in press).

Jansson, S.L., 1958. Tracer studies on nitrogen transformations in soil with special attention to mineralization - immobilization relationships. Kungl. Lantbrukshögskolans Annaler 24: 101-361.

Mills, H.A., A.V. Barker, and D.N. Maynard, 1974. Ammonia volatilization from soil. Agronomy Journal 66: 355-358.

Paul, E.A., and J.A. van Veen, 1978. The use of tracers to determine the dynamic nature of organic matter. Transactions of the 11th International Congress of Soil Science 1978, Vol. III, 61-102.

Van Veen, J.A., 1977. The behaviour of nitrogen in soil. A computer simulation model. Ph. D. Thesis. Vrije Universiteit, Amsterdam.

Van Veen, J.A., W.H. McGill, H.W. Hunt, M.J. Frissel, and C.V. Cole, 1980. Simulation models of the terrestrial nitrogen cycle. In: Clark, F.E. & Rosswal, T. (Eds.). Nitrogen cycling in terrestrial ecosystems. Processes, ecosystem strategies and management impacts. Ecological Bulletins (Stockholm) (in press).

4.7 Use of tracers and computer simulation techniques to assess mineralization and immobilization of soil nitrogen

N.G. Juma and E.A. Paul

1. NAME OF MODEL

TRAMIN - Use of tracer and computer simulation techniques to assess mineralization and immobilization of soil nitrogen.

2. SYSTEM MODELED

The model describes the mineralization and immobilization of soil nitrogen during microbial growth and decay under laboratory conditions.

3. OBJECTIVES

The objectives of this investigation were to develop and test concepts of microbial growth and decay in soil and to study the mineralization and immobilization of soil N using tracer and computer simulation techniques.

4. TIME SCALE

The programme was designed to simulate the duration of the laboratory experiments which lasted from 42 to 84 days. The time resolution was fixed at 0.01 day.

5. DIAGRAM

The flow chart for transfer of C and N involved in the mineralization and immobilization processes is presented in Fig. 1. Four versions of the model are available depending on whether tracer ^{15}N and/or ^{14}C were used. In the basic version, C and N behavior in the mineralization-immobilization processes were simulated. In the other versions, the number of N and/or C integrals were doubled when ^{15}N and/or ^{14}C tracers were used.

6. LEVELS

See 7.

7. GOVERNING EQUATIONS

In models that describe soil organic matter turnover, the microbial biomass transforms C substrates in soil (Paul and Van Veen, 1978) and is directly involved in the N mineralization-immobilization processes. Microbial growth is primarily limited by substrate and nutrient availability and by the physical conditions prevailing in soil. Soil microorganisms grow on a variety of C substrates. For simulation purposes, the exogenous sub-

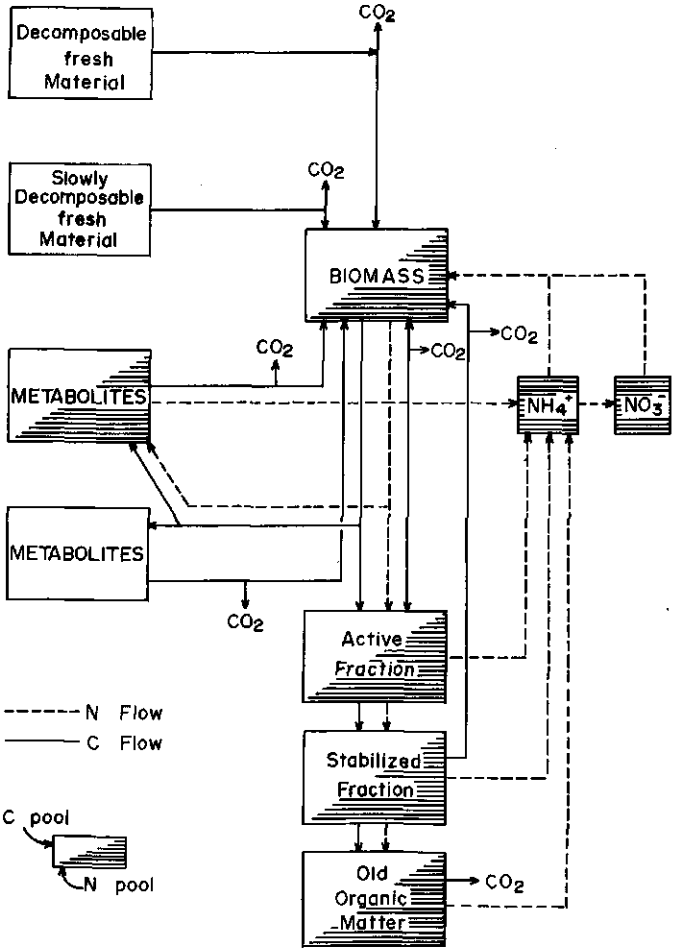


Fig. 1. Flow chart for transfer of C and N involved in the mineralization and immobilization processes.

strates added to soil can be adequately divided into the following categories: (1) decomposable fresh materials consisting of simple carbohydrates; (2) slowly decomposable fresh materials such as cellulose and hemicellulose; (3) materials containing C and N such as proteins, amino sugars, and other nitrogenous compounds; and (4) complex materials such as lignin. In the model, the soil C and N substrates were divided into active-(C+N), stabilized-(C+N) and old-(C+N) (Fig. 1). The techniques and assumptions used to determine the pool sizes are described elsewhere (Paul and Juma, 1980) and are summarized in Table 1.

The concept of an active and a passive organic N phase (Jansson, 1958) was incorporated into the model. The active organic N phase was divided into three components: biomass, active-(C+N) and metabolite-(C+N). This was possible as the biomass and active N can be

Table 1. Initial values of N pools and techniques used for pool size determination.

Pool	^{14}N	^{15}N	Technique
	($\mu g\ g^{-1}$	soil)	
Biomass	167	0.072	Fumigation incubation
Active fraction and metabolites	389	0.169	Isotopic dilution and curve peeling
Old fraction	2073	0	Associated with old carbon (carbon dating)
Stabilized fraction	1496	0	By difference

measured using the techniques summarized in Table 1. The passive organic N phase was divided into two components: stabilized N with a half life of ∿35 years and old N with a half life of ∿600 years. The dynamics of the mineralization processes are presented below:

a. *Microbial growth and N immobilization*

The dynamics of microbial growth and N immobilization were described by first-order kinetics. In most cases, the decomposition of C substrates is independent of microbial biomass size. In the model, the decomposition of C from any pool occurred if C was present in that pool and mineral N was not equal to zero. Thus,

$$dCX/dt = KX \cdot CX \cdot WCOF \cdot TCOF \qquad (1)$$

where

dCX/dt = the rate of substrate decomposition (mg g^{-1} soil d^{-1})

KX = the decomposition rate constant for substrate CX (d^{-1})

CX = the substrate C pool size (mg C g^{-1} soil)

WCOF and TCOF = moisture and temperature reduction factors for sub-optimal conditions. The values of these reduction factors ranged from 0 to 1 depending upon the physical conditions prevailing in soil (Van Veen, 1977).

The rate of C incorporation into the microbial biomass (CXINC; mg C g^{-1} soil d^{-1}) was

$$CXINC = (YCOFX/100) \cdot dCX/dt \qquad (2)$$

where YCOFX is the efficiency of utilization of CX. The rate of CO_2-C evolution ($CXCO_2$, mg C g^{-1} soil d^{-1}) during the decomposition of CX was:

$$CXCO_2 = (1 - (YCOFX/100)) \cdot dCX/dt \qquad (3)$$

The rate of N incorporation into the microbial biomass (CNINC, mg N g^{-1} soil d^{-1}) was

$$CNINC = (dCX/dt)/CNB \qquad (4)$$

where CNB is the C:N ratio of the microbial biomass. Thus, the rate of N uptake during microbial growth was equal to the gross immobilization rate.

b. *Microbial biomass decay*

The decay of the biomass was described by first-order kinetics, i.e. the amount of biomass that decayed per unit time was proportional to its size. The decay C and N products were transferred into the active (C+N) and metabolite pools. The metabolites were divided into two classes: those containing C and N (proteins, amino sugars) and those containing C only (polysaccharides).

In the model, 50% of C and N of the microbial decay products were channelled into the active (C+N) pool. The remainder of the N was channelled into the metabolite (C+N) pool. The amounts of the C entering the metabolite (C+N) and metabolite C pools were calculated as follows:

Assuming a C:N ratio of three, the amount of C transferred to metabolite (C+N) pool was three times the amount of N transferred into it. The remainder of the C [50% of the total microbial C decay products minus C transferred into metabolite (C+N)] was channelled into metabolite-C pool.

c. *Mineralization of N*

Mineralization of N occurred during the decomposition of substrates containing C and N. The rate of N mineralization was calculated by multiplying the rate of C decomposition by the C:N ratio of the pool. Alternately, the rate of N mineralization was calculated by multiplying the decay rate constant (d^{-1}) for the (C+N) pool by the N content of the pool (mg N g^{-1} soil). The gross N mineralization rate was equal to the sum of the rates of N mineralization from various (C+N) pools.

d. *Stabilization of C and N*

Part of the active-(C+N) is transformed physically or chemically into the stabilized-(C+N). Further transformation of the stabilized-(C+N) results in the formation of recalcitrant organic matter. The amounts transferred from one pool to another were described by first-order kinetics.

8. INPUT PARAMETERS

The initial values, decay and transfer rate constants, efficiency of utilization of C substrates and C:N ratios of various (C+N) integrals needed in the model are summarized in Table 2.

Temperature and moisture content were time-dependent variables.

9. OUTPUT VARIABLES

The basic version of TRAMIN evaluates the following variables that are experimentally verifiable: biomass C and N, mineral N and CO_2-C released during incubation. When tracer ^{15}N is used, the following additional variables are verifiable: biomass ^{15}N, mineral ^{15}N,

Table 2. Initial values, decay and transfer rate constants, efficiency of utilization of C substrates and C:N ratios of various (C+N) integrals used in the model.

Pool	C	^{14}N	^{15}N	Decay rate constant	Efficiency of utilization of C	C:N ratio
	($\mu g\ g^{-1}$ soil)		($ng\ g^{-1}$ soil)	(d^{-1})	(%)	
Biomass	1,000	167	72	0.0143	-	6
Active fraction[1]	2,302	384	167	0.0037	40	6
Metabolite-C	15	-	-	1.0	60	-
Metabolite-(C+N)	15	5	2	1.0	60	3
Stabilized-(C+N)[2]	17,542	1,496	0	$6.0 \cdot 10^{-4}$	40	11
Old-(C+N)	24,455	2,073	0	$3.0 \cdot 10^{-6}$	-	11.8
Decomposable C	2	-	-	1.0	60	-
Slowly decomposable C	50	-	-	0.1	60	-
Mineral N	-	21	9	-	-	-

1. Transfer rate constant of active material to stabilized fraction = $0.5 \cdot 10^{-3}$ (d^{-1}).
2. Transfer rate constant of stabilized fraction to old fraction = $3.0 \cdot 10^{-6}$ (d^{-1}).

active ^{15}N and active ^{14}N. The model calculates the size of N integrals and their atom % abundances.

When ^{14}C is used, the following variables are verifiable: biomass ^{14}C, $^{14}CO_2$-C, active ^{14}C (sum of active (C+N), metabolite C and metabolite (C+N)). The model calculates the size of C integrals and their specific activities.

When ^{14}C and ^{15}N are used all the above mentioned variables are verifiable.

10. OBSERVATIONS

Enriched ^{15}N soil samples were obtained from a field experiment conducted on Weirdale loam, a Gray-Black Chernozemic soil. These surface samples were incubated in the laboratory for 12 weeks at field capacity moisture content and 28±1 °C. During the incubation, total N, biomass N, active N and mineral N and their atom % ^{15}N abundances were determined. Also, biomass-C and CO_2-C evolved were measured. Detailed experimental procedures are summarized elsewhere (Paul and Juma, 1980).

The TRAMIN programme was used to simulate the ^{14}N, ^{15}N and C transformations.

11. COMPARISON OF RESULTS

The predicted values of total organic ^{15}N remaining in soil and cumulative CO_2-C evolved were slightly higher than the experimental values (Table 3); the mineral ^{15}N level predicted was lower than the actual value. The other outputs were similar indicating that the gross, transfer rate constants and pool sizes used (Table 2) were of proper magnitude.

The dynamics of various ^{14}N and ^{15}N pools as predicted by the model are shown in Table 4. During the 12 weeks incubation, when no exogenous C was supplied, the biomass with an initial size of 72 ($ng\ g^{-1}$) immobilized 56 ng $^{15}N\ g^{-1}$ soil and decayed by 76 ng^{-1} resulting in a final size of 53 $ng\ g^{-1}$ (Fig. 2). The metabolite N mineralized rapidly and constituted

Table 3. Comparison of experimental data with simulation model outputs at the end of 12 weeks incubation.

Pool	Experimental	Simulated
	($\mu g\ g^{-1}$ soil)	
Total organic ^{15}N remaining in soil	0.203	0.211
Biomass-^{15}N	0.052	0.053
Active fraction + metabolite-^{15}N	0.152	0.150
Stabilized-^{15}N fraction	-	0.007
Mineral-^{15}N	0.045	0.039
Mineral-^{14}N	115	121
Cumulative CO_2-C evolved	938	1153

Table 4. Dynamics of various N fractions in soil during 12 weeks incubation.

Fraction	Simulated values				Experimental value at end of 12 weeks
	Inital size	Inputs	Outputs	Size at end of 12 weeks	
^{15}N (ng g^{-1} soil)					
Biomass-N	72	56	76	53	52
Metabolite-N	2	38	39	1	152
Active-N	166	38	54	150	-
Stabilized-N	0	7	0.1	7	-
Old-N	0	0	0	0	-
Mineral-N	9	86	56	39	45
^{14}N ($\mu g\ g^{-1}$ soil)					
Biomass-N	167	163	187	143	152
Metabolite-N	5	94	98	1	-
Active-N	384	94	125	352	-
Stabilized-N	1496	15	55	1456	-
Old-N	2073	0.1	0.4	2073	-
Mineral-N	21	263	163	121	115

only a small pool at any time. The active N with an initial size of 166 ng $^{15}N\ g^{-1}$ increased by 38 ng g^{-1} and released 54 ng resulting in a final size of 150 ng g^{-1}. A small portion (7 ng g^{-1}) of the ^{15}N released from active-N was transferred to the stabilized fraction while the rest was mineralized. At the end of the 12 weeks incubation, the ^{15}N content of the stabilized-N showed a net increase while the ^{15}N content of biomass and active N showed a net decrease. During the 12 weeks incubation, the model predicted a net mineralization of 30 ng g^{-1} ^{15}N. The relative net changes of the ^{15}N pools expressed as a fraction of ^{15}N mineralized were biomass (-63%), active-N (-53%), metabolite-N (-3%), stabilized-N (+23%), old-N (0%). At present, it is not possible to measure the ^{15}N in stabilized-N and old-N.

During the 12 weeks incubation, the biomass with an initial size of 167 μg $^{14}N\ g^{-1}$ soil immobilized 163 μg g^{-1} and decayed by 187 μg g^{-1} resulting in a net decrease of 24 μg g^{-1} (Fig. 3). The metabolite-N and active-N with equal inputs also declined. The stabilized-N showed a net mineralization of 40 μg g^{-1} while the old N contributed 0.3 μg g^{-1}. Gross

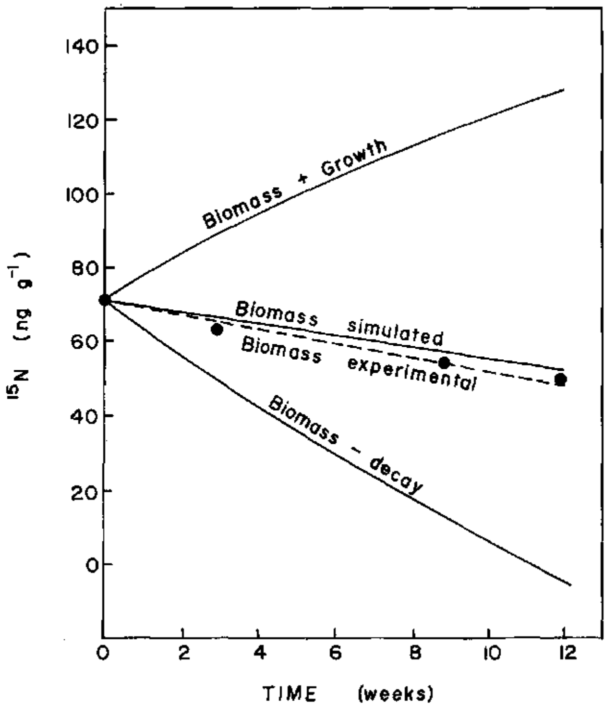


Fig. 2. Biomass-^{15}N: cumulative growth and decay rates.

mineralization during this period amounted to 263 μg g^{-1}, while the net mineralization was 100 μg N g^{-1}. The relative net contribution of N fractions to mineral ^{14}N were biomass (24%), metabolites (4%), active-N (32%), stabilized-N (40%), old-N (0.3%). At present, it is not possible to determine the sizes of metabolite-N, active-N, stabilized-N and old-N.

The turnover time of any pool can be calculated from the tracer data provided the system is in steady state conditions. The soil system generally is not in a steady state condition on a short term basis. Therefore, it is necessary to use simulation techniques to get a good estimate of the fluxes in and out of various pools. In the present version of the TRAMIN model, the C, ^{14}N and ^{15}N transformations were simulated. The major advantage of simulating the N isotopes separately is that it helps to quantify these fluxes accurately. For any pool, the ^{14}N is a good indication of changes in size while the ^{15}N is an excellent index of the activity within the pool. Sensitivity analysis showed that the decay or transfer rate constants used in the model had a very narrow range of values.

Jansson (1958) showed that mineralization and immobilization of N were continuous processes and demonstrated the internal cycling of N. The model predicted that ^{15}N in soil undergoes rapid turnover. During the 12 weeks incubation, 36% (86 ng g^{-1}) of the ^{15}N initially present in soil was mineralized while 23% (56 ng g^{-1}) was reimmobilized. The net change of 30 ng g^{-1} was ∿13% of the total ^{15}N at the beginning of the experiment. Thus,

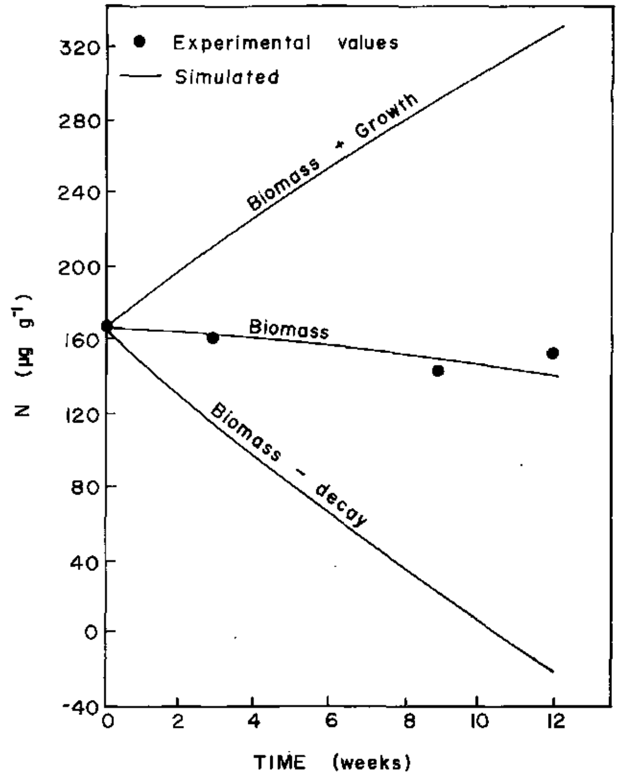


Fig. 3. Total microbial biomass-N: cumulative growth and decay rates.

net mineralization was 1/3 of the gross mineralization, i.e. of every 3 units of N that were mineralized, 2 were reimmobilized, resulting in a net mineralization of 1 unit. Therefore, the half life of ^{15}N in soil organic matter is very long due to the internal cycling of N.

Jansson (1958) suggested that the active organic N phase was the major source of mineralized N. Stanford and Smith (1972) used long term incubations and mathematical techniques to estimate the size and decay rate constant of the mineralizable N pool for 39 soils which were in net mineralization conditions. Thus, the decay rate constant they obtained was related to net mineralization only. The TRAMIN model after considering gross mineralization and immobilization rates predicted that all the N fractions in soil contributed to the mineral N. In this study the active organic N phase comprised of the biomass, active-N and metabolic-N and accounted for almost all of the ^{15}N mineralized, but contributed $\sim$60% of the ^{14}N mineralized. The stabilized-N and old-N accounted for the rest of ^{14}N mineralized. The model predicted that various organic N pools are mineralizable and have different mineralization rate constants. Therefore, it is difficult to describe the soil processes involved in N mineralization by a single first-order decay equation, especially when a net mineralization rate constant is used in the equation.

12. LIMITS AND LIMITATIONS

The model assumes aerobic conditions at all the times and does not consider nitrification or N losses and gains. The N in soil was divided into biomass, active-N, metabolite-N, stabilized-N and old-N, although it is well known that the N compounds in soil form a continuum from simple soluble to recalcitrant compounds. These compounds were grouped into the above mentioned pools based on the decay rates of the pools as determined by tracer and isotopic dilution techniques. At present, it is not possible to measure the size and decay rate constants of the stabilized-N and old-N, however, a wealth of information exists in the literature which supports the concept that large pools or fractions with long half lives exist (Oades and Ladd, 1977).

The mineralization process described in the model assumes that when a substrate containing C and N is decomposed, the N is first converted to NH_4^+. Thus, compounds like simple amino acids and amino sugars are deaminated before being taken up by the biomass. The amount of N immobilized is governed by the amount of C incorporated into the biomass and by the C:N ratio of the biomass.

13. COMPUTER

IBM 360/370.

14. PROGRAMME LANGUAGE

CSMP III.

15. RUNNING TIME/COST

1.5 CPU minutes, cost $16.00 for simulating 84-day laboratory experiment.

16. USERS

The programme has been recently developed, however, the concepts developed could be applied to other soil systems where the role of micro-organisms is explicitly defined in the mineralization and immobilization of N.

17. DEVELOPERS AND PRINCIPAL CONTACT

Noorallah G. Juma and E.A. Paul
Department of Soil Science
University of Saskatchewan
Saskatoon, Saskatchewan
Canada S7N 0W0

REFERENCES

Jansson, S.L., 1958. Tracer studies on nitrogen transformations in soil with special attention to mineralisation-immobilization relationships. Annals Royal Agricultural College

Sweden 24: 101-361.

Oades, J.M., and J.N. Ladd, 1977. Biochemical properties. In: J.S. Russell & E.L. Greacen (Eds): Soil factors in crop production. University of Queensland Press, St. Lucia. p. 127-160.

Paul, E.A., and N.G. Juma, 1980. Mineralization and immobilization of nitrogen by microorganisms. In: F.E. Clark and T. Rosswall (Eds): Terrestrial Nitrogen Cycles. Ecol. Bull. (Stockholm) (in press).

Paul, E.A., and J.A. van Veen, 1978. The use of tracers to determine the dynamic nature of organic matter. Transactions 11th International Congress Soil Science (Edmonton, Alberta) 3: 61-102.

Stanford, G., and S.J. Smith, 1972. Nitrogen mineralization potentials of soils. Soil Science Society of America Proceedings 36: 465-472.

Van Veen, J.A., 1977. The behaviour of nitrogen in soil. A computer simulation model. Ph.D. Thesis, Vrije Universiteit, Amsterdam.

4.8 Plant-soil system of an old Scots pine forest in Central Sweden

E. Bosatta

1. NAME OF MODEL

N1NIT

2. SYSTEM MODELLED

The plant-soil system (mor layer) of an old Scots pine (*Pinus sylvestris* L.) forest in Central Sweden.

3. OBJECTIVE

A great deal is known about separate nitrogen transfer processes in soil. The model is an attempt to synthesize some of the existing hypotheses on how nitrogen mineralization, transport, adsorption and uptake by plant roots are regulated. The model was applied to the mor layer of a forest site (Bosatta et al., 1980), for which a reasonably complete set of empirical data exists on climate, soil processes and components. The aim was to study whether such an integrated model can accurately simulate nitrogen transfers to and from the soil solution, as far as it can be tested from measured data and to identify possible functions in the system which are less satisfactorily described at present. The basic objective was to get an improved background as a basis for further studies on how soil factors regulate plant nutrient uptake.

4. TIME SCALE

Time span: one year.

Time resolution: one day.

5. DIAGRAM

See Fig. 1.

6. LEVELS

The litter and humus (FH) layers are combined, forming one functional structure. Decomposers are considered to utilize this structural substrate, which is made up of two substrates that are divided over three pools:

C_1 = organic carbon in C-N compounds (substances such as proteins, which contain nitrogen as a molecular constituent)

C_2 = organic carbon in C-C compounds (such as cellulose)

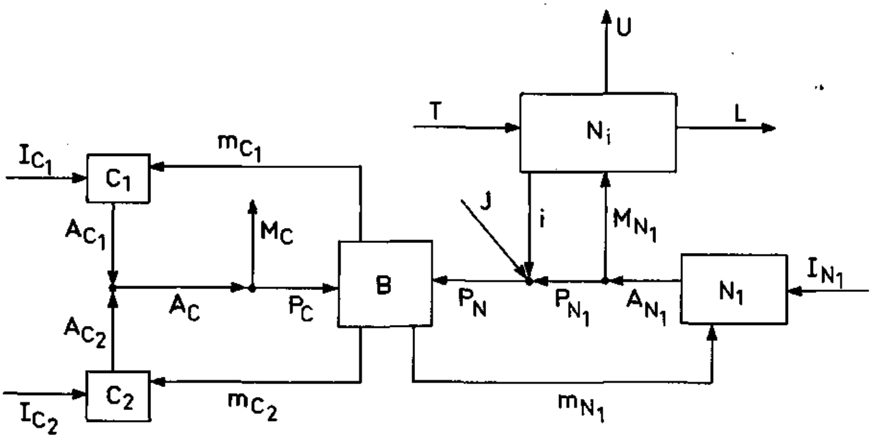


Fig. 1. Flow diagram of nitrogen and carbon in the soil.
N_1, N_i = organic and inorganic nitrogen pools, C_1 = organic carbon bound to organic nitrogen, C_2 = organic carbon not bound to nitrogen, B = decomposer biomass.
I_{C1}, I_{C2}, I_{N1} = rate of input of each element through litter fall and root litter formation.
A_{C1}, A_{C2}, A_{N1}, A_C = decomposition rate of each element and of total carbon.
P_C, P_N, P_{N_1} = incorporation rate in biomass of total carbon, total nitrogen and organic nitrogen.
M_C, M_{N1} = mineralization rate of carbon and nitrogen.
m_{C1}, m_{C2}, m_{N1} = decomposer mortality rate in terms of carbon and nitrogen.
J = nitrogen fixation rate, i = nitrogen immobilization rate.
T, L, U = rates of throughfall, leaching and uptake by roots, respectively, in terms of nitrogen. The sums of flows going out from one point must equal the sum of flows coming in: so, for example, $A_C = A_{C_1} + A_{C_2}$ must be satisfied at all times (from Bosatta, 1980).

N_1 = organic nitrogen in C-N compounds.

In the litter, the whole of the organic nitrogen is included in N_1. However in the humus, nitrogen associated with lignin is considered stable and is not included in the model. The mineral nitrogen compartment (N_i) includes adsorbed ammonium ions and ammonium in the soil solution.

The five compartments are expressed in units of g m^{-2}.

7. GOVERNING EQUATIONS

The model comprises three sub-models:

1. DECOM which deals with processes such as mineralization, decomposition, assimilation, production of decomposer biomass, immobilization.
2. INORG which deals with adsorption of nutrients to soil particles, exchange, leaching.
3. ROOT which deals with uptake of nutrients by the root system.

To test different hypotheses alternative versions of a module have sometimes been used in the model.

Four driving variables are common to all sub-models: D_1 = soil temperature (°C), D_4 = water content (volume fraction of water), D_7 = water infiltration ($1\ m^{-2}\ d^{-1}$) and D_8 = water percolation ($1\ m^{-2}\ d^{-1}$).

DECOM *sub-model*

The theory of Parnas (1975) on the substrate exploitation strategy of decomposers has been adopted for this model. The parameters are (Table 2): G_m = specific production rate of decomposers in a reference state (d^{-1}), f_C = C content of decomposer biomass (mass fraction in dry matter), f_N = N content of decomposer biomass (mass fraction in dry matter), e = efficiency of carbon utilization in decomposers' biomass production (production/assimilation ratio), d_B = specific mortality rate of decomposers (d^{-1}), φ = fraction of decomposers' biomass fixing nitrogen, Q = Q_{10} factor of temperature response of decomposer production rate, and r_c = 'critical' carbon-nitrogen ratio = $f_C/(f_N e)$. Two auxiliary variables are:

$r(t) = (C_1+C_2)/N_1$ the carbon-nitrogen ratio of the decomposing substrate and
$r_1(t) = C_1/N_1$ the carbon-nitrogen ratio of the C-N compounds in the substrate.

The specific production rate, G (d^{-1}), of decomposers is:

$$G = \begin{cases} G_m S\ (D_4)\ Q^{(D_1-20)/10} \\ 0 \quad \text{if carbon or nitrogen is depleted} \end{cases} \tag{1}$$

where $S(D_4)$ is the function shown in Fig. 2. From Equation (1), the specific rate will be equal to G_m when D_1 = 20 °C and D_4 is in the optimal range (0.15–0.25).

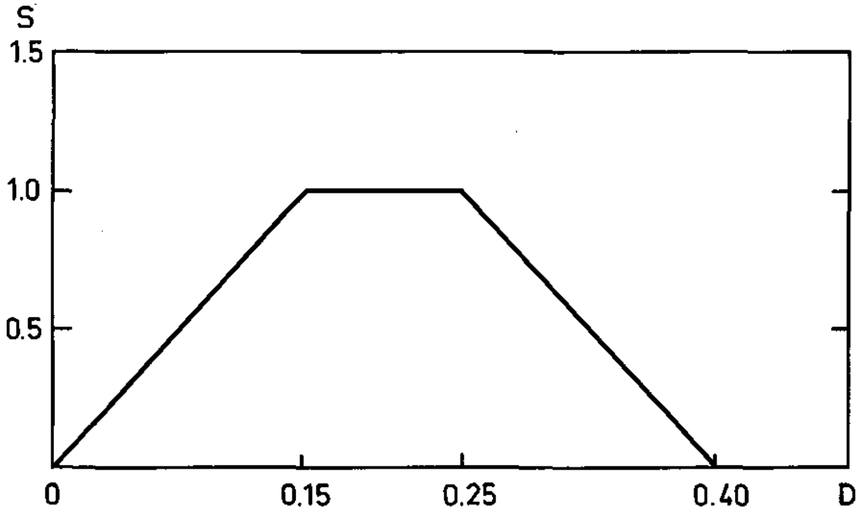


Fig. 2. The moisture scale function, $S(D_4)$, regulating decomposers specific production rate.

The rate of production of dry biomass, P (g m^{-2} d^{-1}), is defined as:

$$P = GB \tag{2}$$

Therefore the incorporation rate of carbon, P_C, and the incorporation rate of nitrogen, P_N, are:

$$P_C = f_C GB \tag{3a}$$

$$P_N = f_N GB \tag{3b}$$

The nitrogen fixation (N_2 fixation) rate, J (g m^{-2} d^{-1}), is defined as:

$$J = \varphi f_N GB \tag{4}$$

i.e., the required amount of nitrogen, P_N, times the fraction, φ, of biomass fixing nitrogen. The remaining nitrogen, P_N-J, must be partly supplied by the inorganic pool, N_i. Therefore the nitrogen immobilization rate is:

$$i = (P_N - J)N_i/(N_i + N_1 D_4) \tag{5}$$

Note that not all N_1 is assumed to be equally available for incorporation as N_i, and that the factor defining this availability has been assumed equal to D_4, i.e., the fraction of the volume filled with water. The incorporation rate of organic nitrogen is (Fig. 1):

$$P_{N_1} = P_N - J - i \tag{6}$$

The decomposition rate of carbon is:

$$A_C = P_C/e = f_C GB/e \tag{7}$$

and the respiration rate is

$$M_C = A_C - P_C = (1-e)f_C GB/e \tag{8}$$

The decomposition rate A_{C_1} (g m^{-2} d^{-1}) of C_1 is given by Parnas (1975):

$$A_{C_1} = \begin{cases} r_1 P_{N_1} & \text{if } r > r_c \quad (9a) \\ A_C C_1/(C_1 + C_2) & \text{if } r \leq r_c \quad (9b) \end{cases}$$

i.e. when nitrogen is limiting (Equation (9a)), C_1 is decomposed according to the requirements of nitrogen for production; when the energy is limiting (Equation (9b)), C is decomposed according to the requirements of carbon. The C_2 decomposition rate is:

$$A_{C_2} = A_C - A_{C_1} \tag{10}$$

N_1 decomposition rate is:

$$A_{N_1} = A_{C_1}/r_1 \tag{11}$$

and the nitrogen mineralization rate (g m^{-2} d^{-1}) is

$$M_{N_1} = A_{N_1} - P_{N_1} \tag{12}$$

If now A_{C_1} is given by Equation (9a), one can see that from Equation (11), $A_{N_1} = P_{N_1}$ and thus $M_{N_1} = 0$. On the other hand (Equation (9b)), if the system is energy limited, M_{N_1} will be greater than zero.
The mortality rate of decomposers m (g m^{-2} d^{-1}) is:

$$m = d_B B \tag{13}$$

where d_B is the specific mortality rate (d^{-1}). If the carbon-nitrogen ratio of the C-N compounds in the biomass of decomposers is 4, the transfers of carbon and nitrogen to organic matter due to decomposers mortality are given by:

$$m_{C_1} = 4f_N m \tag{14a}$$

$$m_{C_2} = (f_C - 4f_N)m \tag{14b}$$

$$m_{N_1} = f_N m \tag{14c}$$

INORG *sub-model*

The parameters in the INORG sub-model are (Table 2): c_0 = concentration of inorganic nitrogen in throughfall (rainfall reaching forest floor), g_0 = amount of ammonium adsorbed to soil particles when the soil complex is in a given reference state, μ_0 = chemical potential at the reference state, k = slope of the adsorption isotherm curve, and c_r = remaining ion concentration.

The throughfall input rate is defined as:

$$T = D_7 c_0 \tag{15}$$

where D_7 is water infiltration rate (1 m^{-2} d^{-1}) and c_0 is as defined above (g 1^{-1}). Similarly, the rate of leaching is:

$$L = D_8 c \tag{16}$$

where D_8 is the percolation rate ($l\ m^{-2}\ d^{-1}$) and c is the nitrogen concentration in the soil solution ($g\ l^{-1}$) which is, in part, controlled by the exchange processes between ammonium and the remaining ions occurring at the adsorption sites on the soil particles.

The exchange phenomenon is approached as follows: let $g(c,c_r)$ be the amount of inorganic nitrogen adsorbed to soil particles; then the following relation between N_i, c and g (all three, henceforth, expressed in ($meq\ l^{-1}$) must be fulfilled:

$$N_i = D_4 c + g(c,c_r) \tag{17}$$

and can be used to calculate the function c(t) if $g(c,c_r)$ is explicitly defined. The function $g(c,c_r)$, known as the adsorption isotherm, is obtained by measuring the changes in the amount of adsorbed nitrogen, with respect to a reference state, as a function of the chemical potential in the equilibrium solution. Under conditions of chemical equilibrium the adsorption rate equals the desorption rate, i.e., the net rate of adsorption is zero, and in this way the hypothesis that g(t) equals its value at equilibrium $g(c,c_r)$, is equivalent to the adiabatic elimination hypothesis(e.g. Haken, 1977).

The adsorption isotherm is expressed as (e.g. Khanna & Ulrich, 1973):

$$g = g_0 + k(\mu-\mu_0) \tag{18}$$

where g_0 ($meq\ l^{-1}$), μ_0 ($J\ meq^{-1}$) and k ($meq^2\ J^{-1}\ l^{-1}$) are defined as above and the chemical potential, μ, is expressed as:

$$\mu = RD_1\ (3 \ln c^a - 2 \ln \frac{c_r^a}{3} \tag{19}$$

where R is the universal gas constant ($J\ meq^{-1}\ K$). D_1 is temperature (K) and c^a and c_r^a are the chemical activities (dimensionless) of ammonium and remaining ions. These are defined as:

$$c^a = f^a c\ 10^{-3} \tag{20a}$$

$$c_r^a = f_r^a c_r\ 10^{-3} \tag{20b}$$

where f^a and f_r^a, henceforth assumed equal to one, are the activity coefficients ($l\ eq^{-1}$). Since the logarithm term makes it difficult to obtain c directly from Equation (17), this equation is differentiated:

$$dN_i = (D_4 + \partial g/\partial c)\ dc = \beta dc \qquad (21)$$

which gives the change induced in the concentration, dc, by a change dN_i produced in the time interval dt under the assumption that D_4 is kept constant during this interval. In simulations with the model, a value is defined for c at the start and the successive increments are calculated with an equation similar to Equation 21 (for more details see Bosatta & Bringmark, 1976).

b, the linear buffering power of the soil, is the average of β over an interval of concentrations (c_1, c_2). From this and Equations (18), (19) and (21):

$$b = D_4 + \frac{3kRD_1}{c_1-c_2} \ln \frac{c_2}{c_1} = D_4 + b_g \qquad (22)$$

If c_2 and c_1 are fixed at 0.15 meq l^{-1} and 0.0005 meq l^{-1}, respectively, then $b_g \approx 4$ (Table 2). For values of c less than c_1, g(c) is fixed at zero.

ROOT

The parameters are: ρ = root density or specific root length (cm cm^{-3}); a = root radius (cm); d_2 = diffusion coefficient of the ammonium ion in free solution ($cm^2\ d^{-1}$), b_g = a term in the linear buffering power of the soil (see Equation (22)). According to Baldwin (1975), the amount of nitrogen taken up by the roots in a time interval Δt is given by

$$U = [1 - \exp \left[\frac{-2\pi d_2 D_4^2 \Delta t\ \rho}{b \ln (a_e/1.65a)}\right]]\ N_i \qquad (23)$$

where $b = b_g+D_4$, $a_e = (\pi\rho)^{-\frac{1}{2}}$ is the effective radius of the soil cylinder surrounding the root (cm), and N_i is the ammonium pool ($g\ m^{-2}$). If Δt is one day, the term in brackets can be interpreted as the specific rate of nitrogen uptake (d^{-1}) and, therefore, U is the daily rate of nitrogen uptake by the roots ($g\ m^{-2}\ d^{-1}$).

8. INPUT PARAMETERS

Initial values (Table 1)

The estimation of carbon and nitrogen in C-C and C-N compounds and nitrogen associated

Table 1. Initial values of soil components ($g\ m^{-2}$) from simulations with the N1NIT model.

C_1	C_2	N_1	N_i	B
213	659	22.6	0.025	5

C_1 = carbon in C-N compounds, C_2 = carbon in C-C compounds, N_1 = nitrogen in C-N compounds, N_i = inorganic nitrogen and B = decomposers biomass.

to lignin was based on analytical data from Staaf & Berg (1977b) and Berg (unpubl.). Start values on decomposers' biomass are transformed data from Clarholm (1977) for bacteria summed with those for fungi (Bååth & Söderström, 1977). Soil animals were not included as a compartment. Data from Popović (1976) and Bringmark (1980) has been used to estimate N_i.

Table 2. Numerical values and denotations for parameters used in the N1NIT model. Parameters of a purely technical nature are not included.

Module	Symbol	Meaning	Value	Dimension
DECOM				
	f_C	Mass fraction of carbon in decomposer biomass	0.5	
	f_N	Mass fraction of nitrogen in decomposer biomass	0.04	
	e	Production/assimilation ratio	0.2	
	φ	Mass fraction of biomass fixating nitrogen	0.02	
		Mass fraction of nitrogen in litter fall	0.003	
		Mass fraction of nitrogen in root-litter formation	0.006	
		Mass fraction of C_1 in litter fall	0.15	
		Mass fraction of C_1 in root-litter formation	0.15	
		Mass fraction of C_2 in litter fall	0.36	
		Mass fraction of C_2 in root-litter formation	0.36	
	G_m	Specific production rate of decomposers in a reference state	0.08	d^{-1}
	d_B	Decomposer mortality rate	0.017	d^{-1}
	Q_{10}	Response of decomposer production rate to a temperature increase of 10 °C	3.0	
INORG				
	c_0	Input concentration of inorganic nitrogen	0.05	meq l^{-1}
	g_0	Adsorbed at equilibrium	0.03	meq l^{-1}
	μ_0	Chemical potential at equilibrium	-38	J meq^{-1}
	k	Adsorption isotherm slope	0.017	meq^2 l^{-1} J^{-1}
	c_r	Remaining ion concentration	0.14	meq l^{-1}
ROOT				
	ρ	Root density	4.5	cm cm^{-3}
	a	Root radius	0.03	cm
	d_2	Diffusion coefficient	1.3	cm^2 d^{-1}
	b_g	Buffer power	4	

(From Bosatta et al. 1980)

Auxiliary values (Table 2)

Parameters for carbon and nitrogen ratios of different litter inputs (Table 2) are based on chemical analyses on a large number of field samples on different litter components from a representative site. Figures from Bååth & Söderström (1977) on nutrient concentration in fungi were used for the decomposer biomass composition. Parameters describing moisture and temperature response of biomass production rate were taken from the corresponding data for respiration from different substrates in controlled environments (Clarholm, 1977; Rosswall, unpubl.).

Micro-organisms are considered to have a high production/assimilation ratio (e). For mixed populations on a long-term basis a value of 0.4 (Heal & MacLean, 1975) or sometimes higher than 0.5 (Kaszubiak et al., 1977) has been suggested. However, introduction of more than one trophic level will decrease the total efficiency ratio, since each additional level includes respiration losses. When this effect was taken into account the effective production/assimilation ratio was estimated at 0.2.

No measurements exist on maximum production (G_m) or mortality (d_B) rates of decomposers. Instead, it was necessary to determine them from the model's behaviour. Climatic data from 1966 were applied to the model and the two parameters were adjusted to achieve a steady state (Section 10) over one year in the carbon, nitrogen and decomposer biomass components. The year 1966 was selected as the one corresponding best to mean monthly temperature and precipitation data from period 1966-1976.

The adsorption parameters g_0, μ_0, and k have been determined experimentally by equilibration of mor samples with weak salt solutions of different composition. The concentration of other cations (c_r) has been given a value to make ($c_r/3$) equal to the mean value of $c_K \sqrt{c_{Ca}} \sqrt{c_{Mg}}$, measured in water collected by tension lysimeters from the litter layer during 1976. The diffusion coefficient for NH_4 (d_2) has been taken from chemical standard literature.

Root density (ρ) and root radius (a) are calculated as the mean of data from three root samplings at the chosen site (H. Persson, unpubl.). The root density (< 1 mm diameter) obtained for Scots pine has been multiplied a factor 30 to get an estimate of total root density, also including heather and cowberry.

Driving variables

- Litter formation

Annual figures for the root-litter formation and litter fall (Staaf & Berg, 1977a; Flower-Ellis & Olsson, 1978; Persson, unpubl.) and chemical analysis of different litter types (Bringmark, 1977; Berg & Staaf, unpubl.) were used to calculate a mean annual influx of chemical substrates to the soil. A litter-fall regime simplified from Flower-Ellis & Olsson (1978) was used; one-third of the total annual litter fall occurred in spring and two-thirds in early autumn (Fig. 3). Knowledge of the dynamics of root-litter formation is poorly, so that a mean figure for daily input during the period May - October was used.

- Nitrogen in throughfall

A mean concentration of inorganic nitrogen in throughfall from the tree canopy (c_0) was calculated from the amounts of water and nitrogen deposited during 1976 (Bringmark, 1977). The nitrogen deposited on the ground was then obtained by multiplying this concentration with amounts of infiltrating water for each time step (day).

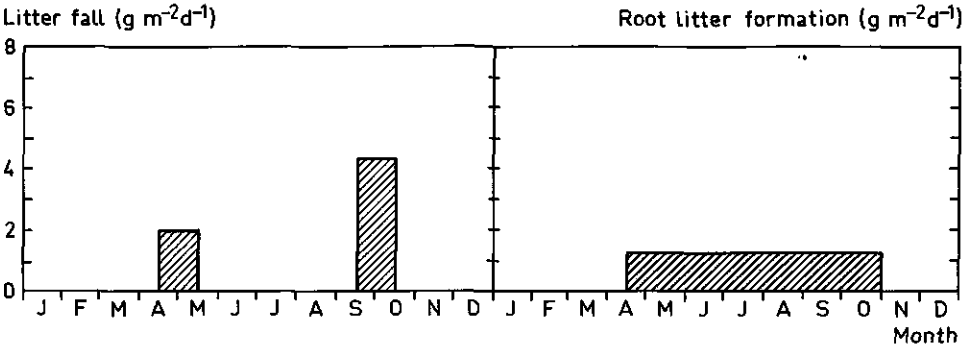


Fig. 3. Litter fall and root-litter formation rates used as driving variables of N1NIT (from Bosatta et al., 1980).

- Soil temperature, water content and water flow

Soil temperatures and data on infiltration, percolation and soil water (Fig. 4) were taken from simulations using SOILW, another model developed at the Swedish Coniferous Forest Project (Halldin et al., 1980). Soil-water data were tested against manual measurements of soil-water content from 1976.

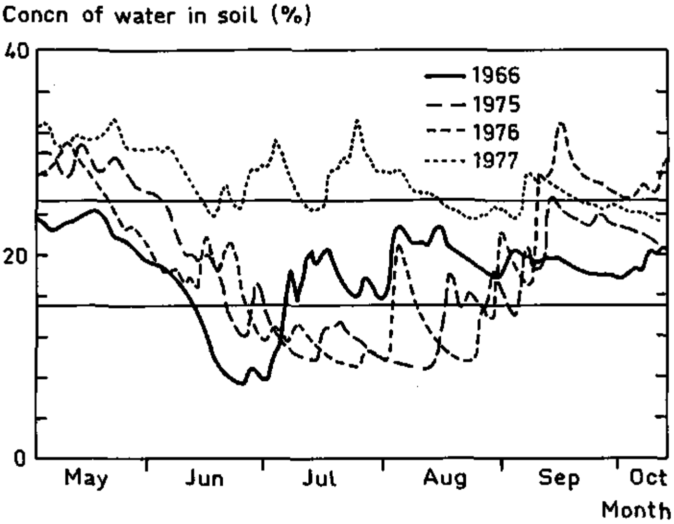


Fig. 4. Daily means of soil-water contents in the FH layer used as driving variables for N1NIT. Horizontal lines indicate optimal range for decomposer production (Bosatta et al., 1980).

9. OUTPUT; VERIFIABLE VARIABLES

All variables shown in Fig. 1 are calculated, plus c, NH_4 concentration in soil solution, g (see Equation (18)) and μ (see Equation (19)).

10 and 11. OBSERVATIONS AND COMPARISON OF RESULTS

Most data comes from measurements carried out in the mor layer of a mature Scots pine stand at Ivantjärnsheden in Central Sweden. The soil is an iron podzol and the mor is made up of a litter layer (mixed with living mosses and lichens) and a humus (FH) layer 5-8 cm and 3-6 cm thick, respectively. Scots pine (*Pinus sylvestris* L.), heather (*Calluna vulgaris* L.), and cowberry (*Vaccinium viti-idaea* L. are the three most important vascular plants on the site, and the trees and undergrowth are well developed. The biomass structure of the latter has been described by Persson (1975). Fine roots (< 2 mm diameter) are mainly distributed in the FH layer (Persson, unpubl.), and plant-nutrient budget calculations (Staaf & Berg, 1977a) indicate that the main part of nitrogen mineralization and uptake in plants occurs there too.

From the history of the stand and its old age, the energy and nutrient flow of the soil is considered approximately balanced. In this study it is treated as a system in a dynamic steady state.

Field data on inorganic nitrogen, decomposer biomass, carbon and nitrogen mineralization and leaching from different years, mainly obtained from 1976 from the mature stand of Ivantjärnsheden (Ih V), were used to test the validity of the model outputs. Unfortunately, uptake in roots in the field cannot be directly measured with existing techniques.

The NH_4 concentration measured in lysimeter leachates during 1976, collected 6 cm below the humus layer (Bringmark, 1980), were of the same magnitude as those produced by the model for concentrations in water within the mor layer (Fig. 5). But the simulated seasonal development of concentrations could not be detected in these lysimeter leachates. Water percolating from the litter to the humus layer showed, however, a very pronounced NH_4 concentration peak in June - July, followed by low concentrations - in the period when simulated values are at a maximum (Fig. 5).

The total amount of inorganic nitrogen (N_i), measured in the field 1974-76 by Popovič (1976, 1977, 1978), was of the same magnitude as the model output. However, the seasonal trend with high peaks in July - August produced by the model was not apparent in the field data on N_i (Fig. 6). Thus, different measurement methods provided contradictory results for the seasonal dynamics of the inorganic nitrogen. The annual differences in Popovič's determinations of N do not agree with values provided by the model (Table 3).

The regulation of decomposer biomass in the model is highly simplified since no mechanistic formulation of consumption is included in it. Instead, a constant specific

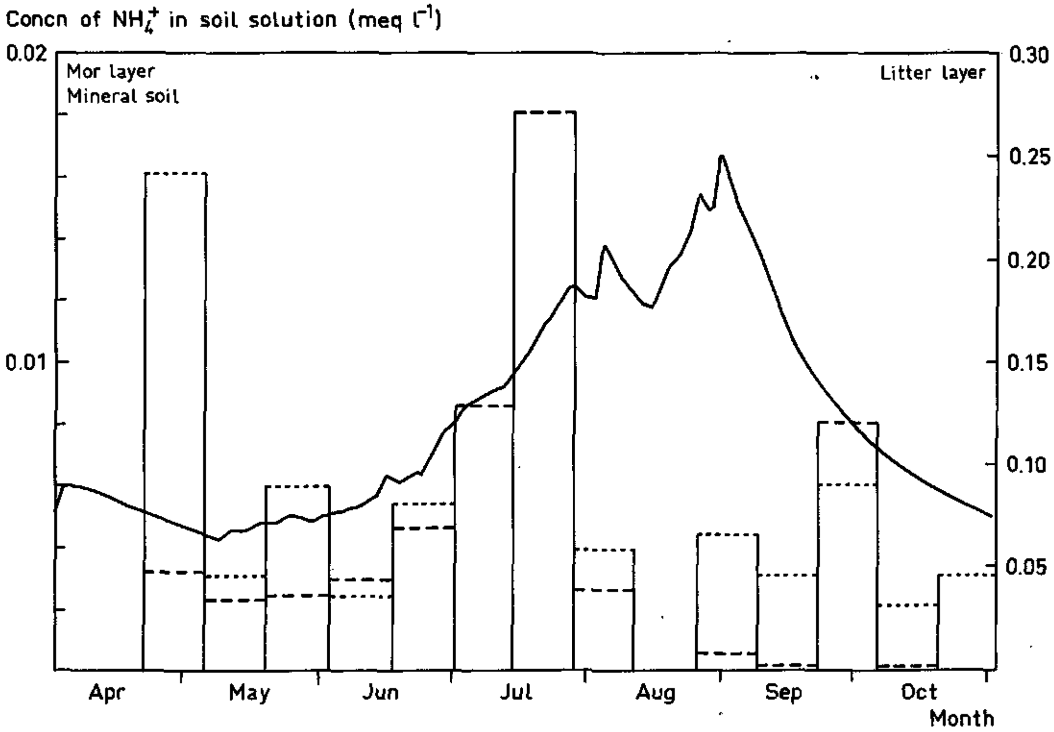


Fig. 5. Comparison of measured and simulated NH_4 concentrations in the soil solution in 1976. The simulated concentrations are daily values for the mor layer (——); the measurements were made bi-weekly in lysimeter leachates from the litter layer (– – –) and in the mineral soil (---) 6 cm below the mor layer (from Bosatta et al. 1980).

Table 3. Amounts of inorganic nitrogen in the mor layer for snow-free periods in 1974-76 simulated by NINIT and measured by KAL $(SO_4)_2$ extraction (Popović, 1976, 1977, 1978).

Year	Simulated inorganic nitrogen (mg m^{-2})	Measured inorganic nitrogen (mg m^{-2})			Number of measurement occasions
		min	mean	max	
1974	31	27	40	67	9
1975	62	15	17	22	4
1976	40	12	19	24	12

(From Bosatta, 1980)

mortality rate is assumed. A simulated regular biomass increase from May onwards to a maximum during September - October followed by a decrease is the general result. Clarholm (1977) reports from 1974 that the highest bacterial biomass was estimated in July - Sep-

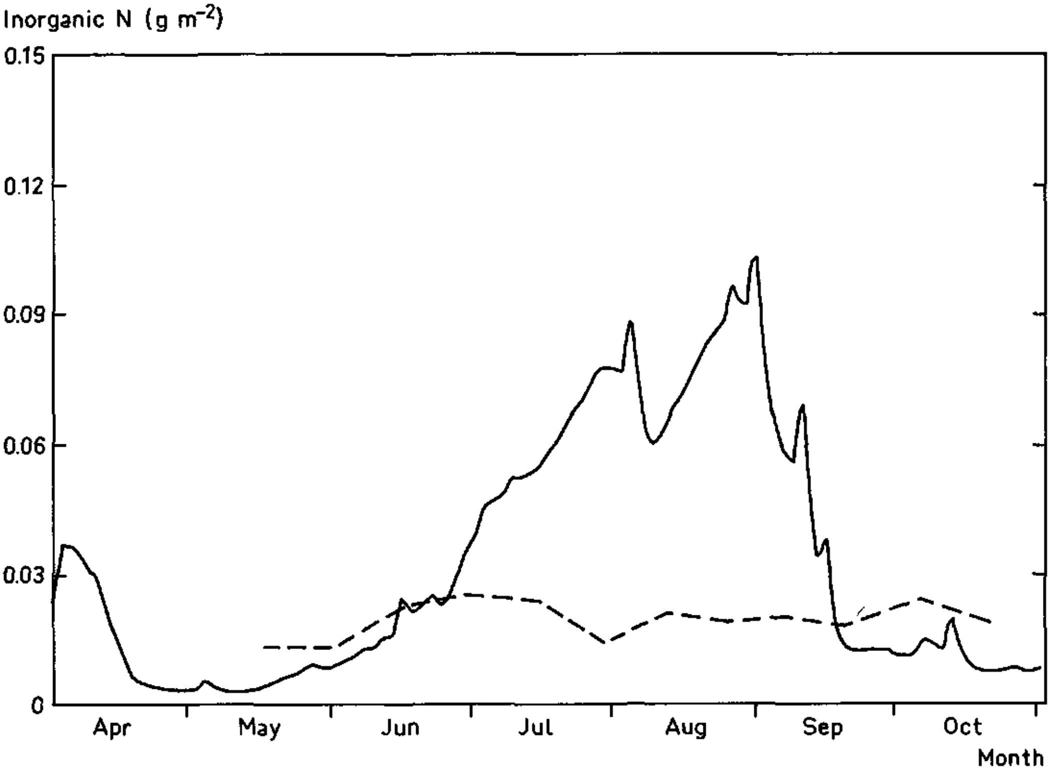


Fig. 6. Total amount of inorganic nitrogen in the mor layer simulated (——) by NINIT and measured (– – –) after extraction using 1% KAL $(SO_4)_2$ on mor samples (Popović, 1978) (from Bosatta et al., 1980).

tember, as apparent from monthly determinations in the A_{01} and A_{02} horizons. A maximum of 10 g m^{-2} was found in September and a minimum of about 2 g m^{-2} in May. During the same period the total fungal biomass was 20-40 g m^{-2} (Bååth & Söderström, 1977). A main problem with these field results is to determine how large a part of the biomass is active. Söderström (1979) found that of 21 samplings during 1975-1977, 2-4% of the total biomass (stained with fluoroscein diacetate (FDA)) was in an active state. The seasonal course of change in active fungel biomass also confirms, in a very rough sense, the model output (Fig. 7), but differences between years do not agree as well.

Realistic field measurements of nitrogen mineralization have proved difficult to perform. Popović (1976, 1977) incubated humus samples from Ih V for six weeks at different times during the years 1974 and 1975. He found the highest capacity of inorganic-nitrogen accumulation in June - July; the model put it slighty later (Fig. 6). The net mineralization of nitrogen (N) for an interval of 6 weeks was measured at less than 30 mg m^{-2}, com-

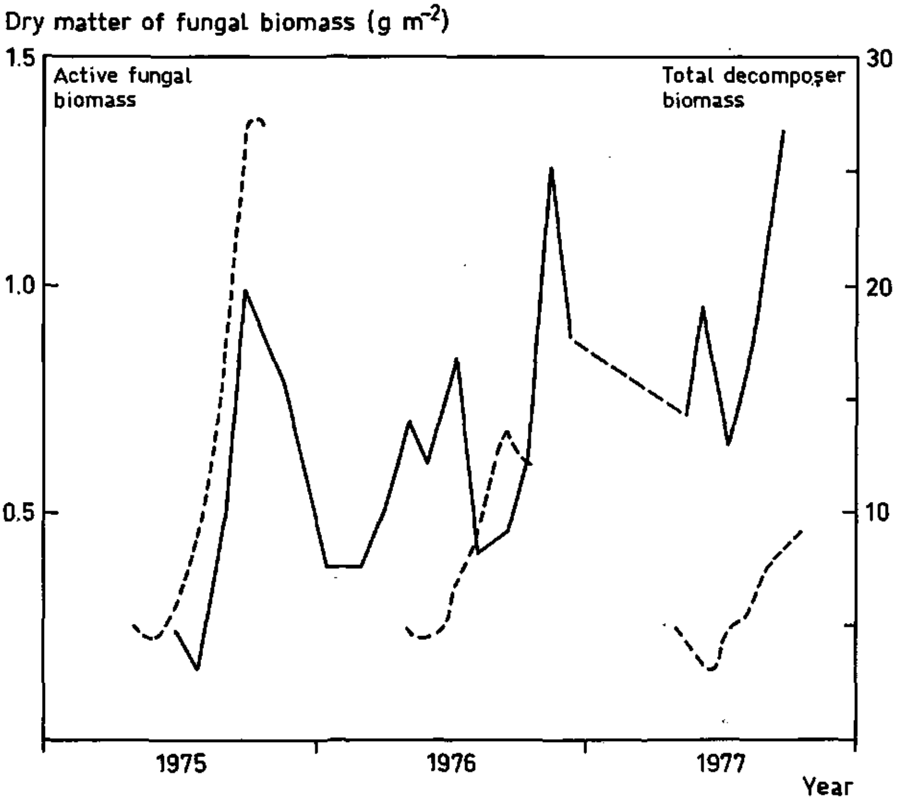


Fig. 7. Total decomposer biomass (---) in the mor layer for 1975-1977 as simulated by NINIT and measured fluoroscein diacetate (FDA)-active fungal biomass (——) (Söderström, 1979) for the same period (from Bosatta et al., 1980).

pared to the mean model output of 6-7 mg m^{-2} d^{-1}. The methodological problems make it difficult to obtain accurate results from field measurements. Thus the data are not very satisfactory for validating the ability of the model to simulate real conditions.

11. COMPUTER

PDP 11/45 - RSX-11M.

12. PROGRAM LANGUAGE

Fortran IV.

Integrations are done using SIMP, a simulation programme developed at the Swedish Coniferous Forest Project (Lohammar, 1979).

13. RUNNING TIME

About 50 seconds.

14. USERS

Internally at the SWECON.

15. DEVELOPER AND PRINCIPAL CONTACT

E. Bosatta, Department of Ecology and Environmental Research, Swedish University of Agricultural Sciences, S-750 07 Uppsala, Sweden

L. Bringmark, and H. Staaf, Department of Plant Ecology, University of Lund, S-223-62 Lund, Sweden.

REFERENCES

Bååth, E., & B.E. Söderström, 1977. Mycelial lengths and fungal biomasses in some Swedish soils, with special reference to a pine forest in Central Sweden. Swedish Coniferous Forest Project Technical Report 13, 45 p.

Baldwin, J.P., 1975. A quantitative analysis of the factors affecting plant nutrient uptake from some soils. Journal of Soil Science 26: 195-206.

Bosatta, E., 1980. Modelling of soil processes - an introduction. In: T. Persson (Ed.): Structure and function of Northern Coniferous Forests. An Ecosystem Study, Ecological Bulletins (Stockholm) (in press).

Bosatta, E., & L. Bringmark, 1976. A model for transport and adsorption of inorganic ions in a pine forest soil ecosystem. A development paper. Swedish Coniferous Forest Project Internal Report 43, 42 p.

Bosatta, E., L. Bringmark, & H. Staaf, 1980. Nitrogen transformations in a Scots pine forest mor. Model analysis of mineralization uptake by roots and leaching. In: T. Persson (Ed.): Structure and function of Northern Coniferous Forests. An Ecosystem Study, Ecological Bulletin (Stockholm) (in press).

Bringmark, L., 1977. A bioelement budget of an old Scots pine forest stand in Central Sweden. Silva Fennica 11: 201-257.

Bringmark, L., 1980. Ion leaching through a podsol in a Scots pine stand. In: T. Persson (Ed.): Structure and function of Northern Coniferous Forests. An Ecosystem Study, Ecological Bulletins (Stockholm) (in press).

Clarholm, M., 1977. Monthly estimations of soil bacterial at Jädraås and a comparison between a young and a mature pine forest on a sandy soil. Swedish Coniferous Forest Project Technical Report 12, 17 p.

Flower-Ellis, J.G.K., & L. Olsson, 1978. Litterfall in an age series of Scots pine stands and its variation by components during the years 1973-1976. Swedish Coniferous Forest Project Technical Report 15, 62 p.

Halldin, S., H. Grip, P-E. Jansson & Å. Lindgren, 1980. Micrometeorology and hydrology of pine forest ecosystems. II. Theory and models. In: T. Persson (Ed.): Structure and function of Northern Coniferous Forests. An Ecosystem Study, Ecological Bulletins (Stockholm) (in press).

Haken, H., 1977. Synergetics. An introduction. Springer Verlag, Berlin-Heidelberg-New York: 320 p.

Heal, O.W., & S.F. MacLean Jr., 1975. Comparative productivity in ecosystems - secondary production. In: W.H. van Dobben & R.H. Lowe-McConnell (Eds.). Unifying Concepts in Ecology, Junk, The Hague and Pudoc, Wageningen, p. 89-108.

Kaszubiak, H., W. Kaczmarek, & Z. Pedziwilk, 1977. Comparison of different methods for estimating the productivity of micro-organisms in soil. Ekologia Polska 25: 289-296.

Khanna, P.K., & B. Ulrich, 1973. Ion exchange equilibria in an acid soil. Göttingen Bodenkünder Berichte 29: 211-230.

Lohammar, T., 1979. SIMP - Interactive Mini-Computer Package for Simulating Dynamic and Static Models. In: S. Halldin (Ed.). Comparison of forest water and energy exchange models. Proceedings from an IUFRO Workshop, Uppsala (Sweden), September 24-30, 1978.

Parnas, H., 1975. Model for decomposition of organic material by micro-organisms. Soil Biology Biochemistry 7: 161-169.

Persson, H., 1975. Dry matter production of dwarf shrubs, mosses and lichens in some Scots pine stands at Ivantjärnsheden, Central Sweden. Swedish Coniferous Forest Project Technical Report 2, 25 p.

Popović, B., 1976. Nitrogen mineralisation in an old pine stand. Swedish Coniferous Forest Project Internal Report 35, 16 p. (in Swedish, English abstract).

Popović, B., 1977. Nitrogen mineralisation in an old and a young Scots pine stand. Swedish Coniferous Forest Project Internal Report 60, 15 p. (in Swedish, English abstract).

Popović, B., 1978. Nitrogen mineralisation during the early phase after clear-cutting. In: U. Granhall (Ed.). Nutrient Turnover in the Early Phase after Clear-cutting. Results from Introductory Investigations. Swedish Coniferous Forest Project Internal Report 70, 40-46 (in Swedish, English abstract).

Söderström, B.E., 1979. Seasonal fluctuations of active fungal biomass in horizons of a podzolized pine forest in Central Sweden. Soil Biology Biochemistry 11: 149-154.

Staaf, H., & B. Berg, 1977a. Mobilization of plant nutrients in a Scots pine forest mor in Central Sweden. Silva Fennica 11: 210-217.

Staaf, H., & B. Berg, 1977b. A structural and chemical description of litter and humus in a mature Scots pine stand. Swedish Coniferous Forest Project Internal Report 65, 31 p.

4.9 Formulation, process controls, parameters and performance of PHOENIX: A model of carbon and nitrogen dynamics in grassland soils

W.B. McGill, H.W. Hunt, R.G. Woodmansee, J.O. Reuss and K.H. Paustian

1. NAME OF MODEL

PHOENIX. For a complete description of the model see 'McGill, W.B., Hunt, H.W., Woodmansee[1], R.G., and Reuss, J.O., 1980. Dynamics of carbon and nitrogen in grassland soils. In: Clark, F.E., and Rosswall, T. (Eds) Terrestrial Nitrogen Cycles: Processes, Ecosystem Strategies and Management Impacts. Ecol. Bull. (Stockholm).

2. SYSTEM MODELED

Transformations and transports of carbon and nitrogen in native grasslands are modeled. The model represents a generalized plant canopy, bacteria, fungi, several organic fractions of carbon and nitrogen, ammonium, and nitrate. Denitrification and plant and microbial respiration are processes that represent gaseous losses. The model has been altered by various means to represent perturbations such as fertilization, plowing, suppression of bacteria or fungi, and addition of cattle wastes.

3. OBJECTIVES

The objective of this research was to explore, through simulation modeling, the relationships among plant processes and microbial processes and their effect on plant production, microbial secondary production, and nitrogen cycling. Our emphasis was on microbes, soil organic matter, and inorganic N, which were modeled more mechanistically than were plants. We required of the plant model primarily that N content and net production respond realistically to changes in the availability of N_i (inorganic nitrogen). Both carbon and nitrogen were treated because of their important interactions.

4. TIME SCALE

Most model components operate on a daily time step. Bacterial and fungal growth processes, however, operate at 0.2 day time steps. The model has been used to simulate system behavior for up to two years.

5. DIAGRAM

Figures 1 and 2 show compartment diagrams for the model. There is one-to-one correspond-

---

[1] This paper reports on work supported in part by National Science Foundation Grant DEB77-07229, Gaseous Losses of Nitrogen from Grassland Systems.

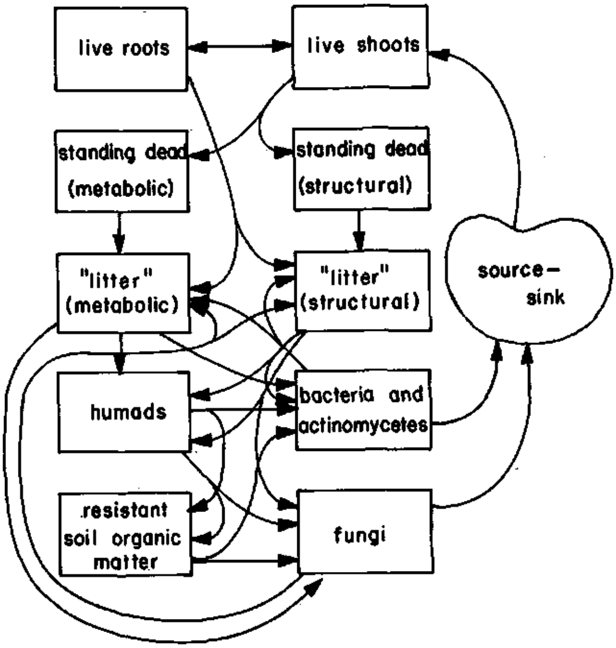


Fig. 1. Compartment diagram for carbon flow. State variables are replicated by depth (0-2, 2-6, 6-14, 14-30 cm).

ence between state variables in the C flow and N flow submodels, except for ammonium and nitrate in the N submodel, and the source-sinks in both models. State variables for belowground portions of the system are replicated in four soil layers. State variables are expressed as g N m^{-2} or g C m^{-2}. The forked arrows in the figure represent flows, calculated as a loss from one compartment, divided, and sent to two compartments. In many cases flows are calculated on the basis of biomass, taken as carbon, with the fraction of N leaving the compartment equal to the fraction of C leaving. The only exceptions are flows of N_2, CO_2 (respiration, and the death of shoots and roots, where the flow of N is relatively less than that of C.

Litter (dead plant parts and dead microbes) is divided into two fractions (Figs. 1 and 2). The structural component is assumed to have a C:N ratio of 150 for plant parts and 30 for microbes. The metabolic component consists of menbranes, organelles, and cytoplasm and is assumed to have a C:N of 5 and 3 for plants and microbes, respectively. The two classes of substrate differ in their availability to microbes, in their C:N ratios, and in their relationship to more resistant substrates (humads and resistant soil organic matter). The C:N ratio of dying material, lying between that of the metabolic component and the structural component, determines a unique split between the two fractions.

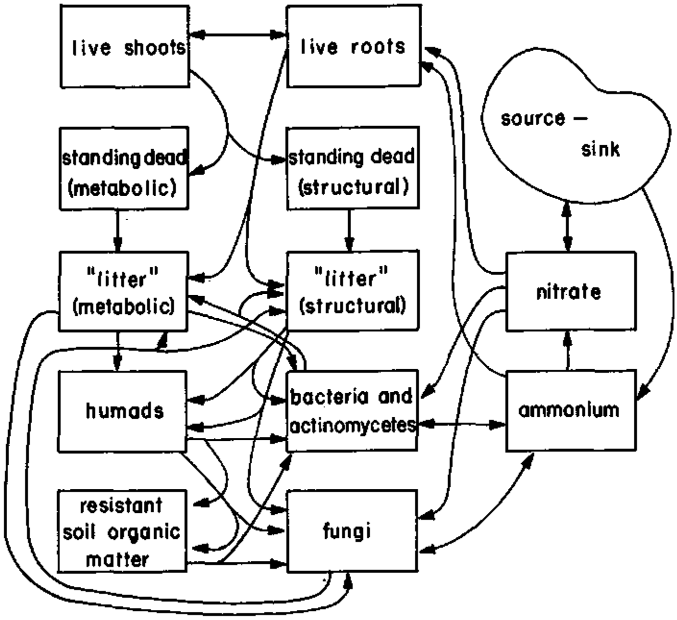


Fig. 2. Compartment diagram for nitrogen flow. State variables are replicated by depth (0-2, 2-6, 6-14, 14-30 cm).

6. LEVELS

See section 5.

7. GOVERNING EQUATIONS

PHOENIX is constructed as a flow-oriented simulation model in which processes or 'flows' between compartments (state variables) are expressed as finite difference equations. Flows are presented as rate equations in algebraic form for purposes of description. The values of the rate equations are used to compute a finite difference solution for the model state variables. Processes are generally modelled by specifying a maximum rate and a series of non-dimensional reduction factors. The reduction factors are formulated as '0 to 1' functions, with the independent variable being an environmental (i.e., temperature, moisture) or biological (i.e., C/N ratio, population density) condition influencing the process. Model flows are in g m^{-2} day^{-1} for each of the soil layers described in the previous section. Model processes are described within the following categories: inputs, decomposition and uptake, respiration, ammonification, nitrification, denitrification, mortality, and leaching.

Inputs

Atmospheric deposition and fertilizer addition are included at a daily time step. Ammonium is added only to the top layer but nitrate, because of its greater mobility, is distributed among all the soil layers.

a. Ammonium input to the top soil layer (daily time step)

$$I_1 = A_1 \cdot P + F_1/DT$$

where

I_1 = NH_4-N g m^{-2} day^{-1}
A_1 = deposition rate (NH_4-N g m^{-2} cm^{-1})
P = precipitation (cm day^{-1})
F_1 = NH_4-N added through fertilization (g m^{-2})
DT = time step (day).

b. Nitrate input to the top soil layer (daily time step)

$$I_2 = D_1 \cdot A_2 \cdot P + F_2/DT$$

where

I_2 = NO_3-N g m^{-2} day^{-1}
D_1 = distribution fraction (non-dimensional)
A_2 = atmospheric deposition rate (NO_3-N g m^{-2} cm^{-1})
P = precipitation (cm day^{-1})
F_2 = NO_3-N added through fertilization (g m^{-2})
DT = time step (day).

c. Nitrate input to each of the second, third, and fourth soil layers (daily time step

$$I_3 = D_2 \cdot A_2 \cdot P$$

where

I_3 = NO_3-N g m^{-2} day^{-1}
D_2 = distribution fraction (non-dimensional)
A_2 = atmospheric deposition (NO_3-N g m^{-2} cm^{-1})
P = precipitation rate (cm day^{-1}).

Decomposition and uptake

Decomposition and uptake processes are modeled separately for each of the two decomposer groups, bacteria/actinomycetes and fungi, considered in the model. However, since the functional forms are the same for both groups, generalized forms of the equations will be described here. Section 8 contains more specific information on the parameters used for each decomposer group.

a. Decomposition of the structural component of litter (daily time step)

$$D = \frac{1}{1 + K_1 \cdot (M/S)^{K_2}}$$

$$SB = T \cdot W \cdot R \cdot M \cdot CN \cdot D$$

where

SB = C g m^{-2} day^{-1}
T = effect of soil temperature on decomposition (non-dimensional)
W = effect of soil moisture on decomposition (non-dimensional)
CN = effect of microbial C:N ratio on decomposition (non-dimensional)
R = decomposition rate constant (day^{-1})
M = microbial biomass (C g m^{-2})
D = effect of microbial density on decomposition (non-dimensional)
S = structural biomass (C g m^{-1})
K_1, K_2 = constants related to substrate particle size (non-dimensional).

Microbial assimilation of C and N from structural decomposition is based on a utilization fraction. The remaining C and N fractions flow to the humad components.

b. Decomposition of humad (daily time step)

$$C_h = P_1 \cdot (H_c/Q)^{P_2}$$

$$HB = T \cdot W \cdot M \frac{V_h \cdot C_h}{K_h + C_h}$$

where

HB = C g m^{-2} day^{-1}
T = effect of soil temperature on humad decomposition (non-dimensional)
W = effect of soil moisture on humad decomposition (non-dimensional)
M = microbial biomass (C g m^{-2})
V_h = maximum rate of humad decomposition (day^{-1})
K_h = half-saturation constant (C mg liter^{-1})
C_h = solution concentration of humads (C mg liter^{-1})
H_c = humad carbon (g m^{-2})

Q = soil water for the layer (ml m^{-2})

P_1, P_2 = parameters determining the solution concentration of humads.

Microbial assimilation of C and N from humad decomposition is based on a utilization fraction. The remaining C and N fractions flow to the resistant soil organic matter component.

c. Decomposition of resistant soil organic matter (daily time step)

$$C_r = R_c/D$$

$$RB = T \cdot W \cdot V_r \cdot M \cdot C_r$$

where

RB = C g m^{-2} day^{-1}

T = effect of soil temperature on the decomposition of resistant soil organic matter (non-dimensional)

W = effect of soil moisture on the decomposition of resistant soil organic matter (non-dimensional)

V_r = decomposition rate constant (m^3 g^{-1} C day^{-1})

M = microbial biomass (C g m^{-2})

R_c = resistant soil organic matter carbon (g m^{-2})

C_r = resistant soil organic matter concentration (C g m^{-3})

D = soil layer depth (m).

Microbes assimilate all the C and N made available by the decomposition of resistant soil organic matter.

d. Decomposition of metabolic litter component (1/5 day time step)

$$C_m = P_1 \cdot (M_c/Q)^{P_2}$$

$$MB = T \cdot W \cdot M \; \frac{V_m \cdot C_m}{K_m + C_m}$$

where

T = effect of soil temperature on the decomposition of the metabolic component of litter (non-dimensional)

W = effect of soil moisture on the decomposition of the metabolic component of litter (non-dimensional)

M = microbial biomass (C g m^{-2})

V_m = maximum rate of metabolic decomposition (day^{-1})
K_m = half-saturation constant (C mg $liter^{-1}$)
C_m = solution concentration of metabolic component (C mg $liter^{-1}$)
M_c = metabolic component carbon ($g\ m^{-2}$)
Q = soil water for the layer ($ml\ m^{-2}$)
P_1, P_2 = paramters determining the solution concentration of the metabolic component.

Microbes assimilate all the C and N made available by the decomposition of the metabolic component of litter.

e. Ammonium uptake (daily time step)

$$C_a = \frac{10^6 \cdot NH_4 \cdot S}{Q}$$

$$U_a = T \cdot W \cdot CN_m \cdot M \cdot \frac{V_a \cdot C_a}{K_a + C_a}$$

where

U_a = $N\ g\ m^{-2}\ day^{-1}$
T = effect of soil temperature on uptake of ammonium (non-dimensional)
W = effect of soil moisture (non-dimensional)
CN_m = effect of microbe C:N ratio (non-dimensional)
M = microbial biomass ($C\ g\ m^{-2}$)
V_a = maximum rate constant for ammonium uptake (day^{-1})
K_a = half-saturation constant (mg $liter^{-1}$)
C_a = solution concentration of ammonium (N mg $liter^{-1}$)
S = fraction of ammonium in solution (non-dimensional)
NH_4 = ammonium ($N\ g\ m^{-2}$)
Q = soil water for the layer ($ml\ m^{-2}$).

f. Nitrate uptake (1/5 day time step)

$$U_n = T \cdot W \cdot CN_m \cdot M \cdot \frac{V_n \cdot C_n}{K_n + C_n}$$

where

T = effect of soil temperature on the uptake of nitrate (non-dimensional)
W = effect of soil moisture on the uptake of nitrate (non-dimensional)
CN_m = effect of microbe C:N ratio on the uptake of nitrate (non-dimensional)

M = microbial biomass (C g m^{-2})
V_n = maximum rate of nitrate uptake (day^{-1})
K_n = half-saturation constant (N mg $liter^{-1}$)
C_n = solution concentration of nitrate (N mg $liter^{-1}$).

Microbial respiration (1/5 day time step)

Release of CO_2 as a result of microbial respiration is modeled for both decomposer groups. The functional form is the same for both, but parameter values are specific for each group. A generalized equation for both decomposer groups is given below.

$$R_m = (1 - Y_m) \cdot U_m + E_m \cdot M \cdot T$$

where

R_m = C g m^{-2} day^{-1}
Y_m = maximum percent yield of uptake carbon (non-dimensional fraction)
U_m = microbial uptake rate of carbon (C g m^{-2} day^{-1})
E_m = maintenance energy requirement constant (day^{-1})
M = microbial biomass (C g m^{-2})
T = effect of temperature on microbial respiration (non-dimensional).

Ammonification (daily time step)

$$AM = T \cdot W \cdot CN_a \cdot M \cdot R_a$$

where

AM = N g m^{-2} day^{-1}
T = effect of soil temperature on ammonification (non-dimensional)
W = effect of soil moisture on ammonification (non-dimensional)
CN_a = effect of microbial C:N ratio (non-dimensional)
M = microbial nitrogen (g m^{-2})
R_a = rate constant for ammonification (day^{-1}).

Nitrification (daily time step)

Nitrification, in the model, includes the oxidation of ammonium used as an energy source by nitrifying bacteria and the 'waste' oxidation of ammonium in the presence of the nitrification enzymes. Principal influences on the nitrification rate include: temperature, moisture, nitrifier population density, and the amount of inhibitory substances present.

a. Formation of nitrification inhibitor

$$I_f = T \cdot W \cdot K_f \cdot R$$

where

I_f = C g m^{-2} day^{-1}
T = effect of temperature on the rate of inhibitor formation (non-dimensional)
W = effect of soil moisture on the rate of inhibitor formation (non-dimensional)
K_f = rate constant for inhibitor formation (day^{-1})
R = root biomass (C g m^{-2}).

b. Decay of nitrification inhibitor

$$I_d = T \cdot W \cdot M \cdot K_d \cdot I_c$$

where

I_d = C g m^{-2} day^{-1}
T = effect of soil temperature on inhibitor decay (non-dimensional)
W = effect of soil moisture on inhibitor decay (non-dimensional)
M = microbial biomass (C g m^{-2})
K = decay rate constant (ml g^{-1} C day^{-1})
I_c = inhibitor solution concentration (C g ml^{-1}).

c. Nitrification

$$NT = T \cdot W \cdot I \cdot \left(M_n \cdot (1 - M_n/M_x) \cdot \frac{(V_n \cdot C_n)}{K_n + C_n} + M_n \frac{(E_n + W)}{K'_n + C_n} \cdot C_n \right)$$

where

NT = N g m^{-2} day^{-1}
T = effect of soil temperature on the nitrification rate (non-dimensional)
W = effect of soil moisture on the nitrification rate (non-dimensional)
I = effect of nitrification inhibitor (non-dimensional)
M_n = nitrifier nitrogen (g m^{-2})
M_x = maximum nitrifier nitrogen (g m^{-2})
V_n = maximum uptake rate (day^{-1})
K_n = half-saturation constant (N mg $liter^{-1}$)
E_n = maintenance energy rate constant (day^{-1})
W = waste energy constant (day^{-1})

K'_n = half saturation constant (N mg liter^{-1})
C_n = solution concentration of NH (N mg liter^{-1}).

Denitrification (daily time step)

$$D = T \cdot W \cdot M \cdot F_d \cdot \frac{V_d \cdot C_n}{K_d + C_n}$$

where

D = N g m^{-2} day^{-1}
T = effect of soil temperature on denitrification (non-dimensional)
W = effect of soil moisture on denitrification (non-dimensional)
M = microbial biomass (g m^{-2})
F_d = fraction of bacteria which are denitrifiers (non-dimensional)
V_d = maximum rate constant for denitrification (day^{-1})
K_d = half-saturation constant for nitrate uptake (N mg liter^{-1})
C_n = solution concentration of nitrate (N mg liter^{-1}).

Microbial mortality (daily time step)

Microbial mortality is modeled as a function of lethal stresses, such as drying and freezing, and a density-dependent death rate due to biotic interactions. Although bacteria and fungal mortality are modeled separately, the functional form described below applied to both groups.

Microbial death rate

$$DM_t = M \cdot (T_m \cdot D_t + W_m \cdot D_w + T \cdot W \cdot D \cdot (1 - M_n/M))$$

where

DM_t = C g m^{-2} day^{-1}
M = microbial biomass (C g m^{-2})
T_m = effect of soil temperature on mortality due to freezing (non-dimensional)
D_t = death rate due to freezing (day^{-1})
W_m = effect of soil moisture on mortality due to drying (non-dimensional)
D_w = death rate due to drying (day^{-1})
T = effect of soil temperature on death rate (non-dimensional)
W = effect of soil moisture on death rate (non-dimensional)
D = density-dependent death rate (day^{-1})
M_n = minimum microbial population level (C g m^{-2}).

Leaching losses

Leaching losses from the surface soil layer are modeled for all soluble materials (NH_4^+, NO_3^-, metabolic component of substrates and humads). The flow is dependent on the material solution concentration and water flow through the soil.

$$L = C_e \cdot WF$$

where

L = nitrogen or carbon leached (g m^{-2} day^{-1})
C_e = solution concentration of the material (g m^{-3})
WF = water flow from layer n to layer n+1 (cm day^{-1}).

8. INPUT PARAMETERS

Initial conditions

Model state variables, shown in Fig. 1 and 2, are initialized in the model data section. All state variable values are in g m^{-2}. Belowground components are divided into four soil layers (D) of 2, 4, 8, and 16 cm depth respectively. Model state variables and their definitions are given below:

X (1)	source-sink
X (2)	shoot carbon (C)
X (3-6)	root C by depth
X (11-14)	bacteria and actinomycetes (C) by depth
X (15-18)	fungi (C) by depth
X (21-24)	resistant component soil organic matter by depth (C)
X (31-34)	humads (C) by depth
X (51-54)	structural component or litter (C) by depth
X (55-58)	metabolic component of litter (C) by depth
X (61)	metabolic component of standing dead (C)
X (62)	structural component of standing dead (C)
X (70)	nitrification inhibitor source-sink
X (71-74)	nitrification inhibitor by depth
X (76-78)	nitrifiers by depth N (C not modeled)
X (79)	source sink for nitrifier N
X (811-14)	nitrate (N) by depth
X (821-23)	ammonium (N) by depth
X (831-34)	humads (N) by depth
X (841-44)	root N by depth
X (851-54)	structural component of litter (N) by depth
X (855-58)	metabolic component of litter (N) by depth

X (860)	shoot N
X (861)	metabolic component of standing dead (N)
X (862)	structural component of standing dead (N)
X (871-74)	bacteria and actinomycetes (N) by depth
X (875-78)	fungi (N) by depth
X (891-94)	resistant component soil organic matter by depth (N)

Auxiliary parameters/process controls

Parameter values used in the model are listed with the FORTRAN-coded variable name, definition, and units. Paremeters used specifically in the producer submodel are not shown.

1. Atmospheric inputs

SRNNC	atmospheric nitrogen deposition rate (g cm^{-1} H_2O)
SSNNC	fraction of deposited N going to the top layer
STNNC	fraction of deposited N going to each of the second, third, and fourth layers

2. Decomposition

ETB	effect of soil temperature on bacterial decomposition and uptake (non-dimensional)
ETF	effect of soil temperature on fungal decomposition and uptake (non-dimensional)
EWB	effect of soil water tension (bars) on bacterial decomposition and uptake (non-dimensional)
EWF	effect of percent soil water on fungal decomposition and uptake
FHTM	fraction of decomposed humads utilized by microbes
FSTM	fraction of decomposed structural litter utilized by microbes
HUBP1	maximum uptake rate constant for humads by bacteria (day^{-1})
HUBP2	half-saturation constant for bacterial humad uptake (C mg liter^{-1})
HUMP1, HUMP2	Freundlich isotherm parameters for calculating the solution concentration of humads
HUMAP	adsorption rate constant for humads of free meatbolic litter material (day^{-1})
LAPT	effect of temperature on the adsorption rate by humads (non-dimensional)
MBP1	maximum rate of decomposition of meatbolic litter component by bacteria (day^{-1})
MBP2	half-saturation constant for decomposition of metabolic litter component by fungi (C mg liter^{-1})
MCP1, MCP2	Freundlich isotherm parameters for calculating the solution concentration of the metabolic litter component
MFP1	maximum rate constant for decomposition of metabolic litter component by fungi (day^{-1})
MFP2	half-saturation constant for decomposition of metabolic litter by fungi (C mg liter^{-1})
RSOB1	rate constant for decomposition of resistant soil organic matter by bacteria (day^{-1})
RSOF1	rate constant for decomposition of resistant soil organic matter by fungi (day^{-1})
SBP1U	rate constant for decomposition by bacteria of structural litter (day^{-1})

SBP2	effect of bacteria C:N ratios on decomposition rate (non-dimensional)
SMP5U, SBP6U	parameters for determining the effect of the bacteria population density on decomposition (non-dimensional)
SFP1U	rate constant for decomposition by fungi of structural litter (day^{-1})
SFP2	effect of fungi C:N ratio on decomposition rate (non-dimensional)
SFP5U, SFP6U	parameters for determining the effect of the fungi population density on decomposition (non-dimensional)

3. Inorganic nitrogen uptake

NHBP1	maximum rate constant for uptake of ammonium by bacteria (day^{-1})
NHBP2	half-saturation constant for uptake of ammonium by bacteria (N mg liter^{-1})
NHFP1	maximum rate constant for uptake of ammonium by fungi (day^{-1})
NHFP2	half-saturation constant for uptake of ammonium by fungi (N mg liter^{-1})
NH4BP	factor relating bacteria C:N ratio to inorganic N uptake rate (non-dimensional)
NH4FP	factor relating fungi C:N ratio to inorganic N uptake rate (non-dimensional)
NOBP1	maximum rate constant for the uptake of nitrate by bacteria (day^{-1})
NOBP2	half-saturation constant for uptake of nitrate by bacteria (N mg liter^{-1})
NOFP1	maximum rate constant for uptake of nitrate by fungi (day^{-1})
NOFP2	half-saturation constant for uptake of nitrate by fungi (N mg liter^{-1})

4. Respiration

MERB	fractional rate of energy required for maintenance by bacteria (day^{-1})
MERF	fractional rate of energy required for maintenance by fungi (day^{-1})
YB	fraction of carbon uptake utilized by bacteria (% yield)
YF	fraction of carbon uptake utilized by fungi (% yield)

5. Ammonification

AMBP1	effect of bacteria C:N ratio on ammonification rate (non-dimensional)
AMBP2	rate constant for ammonification by bacteria (day^{-1})
AMFP1	effect of fungi C:N ratio on ammonification (non-dimensional)
AMFP2	rate constant for ammonification by fungi (day^{-1})

6. Nitrification

FU	joint effect of soil temperature and soil water tension (bars) on nitrification (non-dimensional)
KN	half-saturation constant for ammonium uptake (N mg liter^{-1})
KN2	half-saturation constant for 'waste' oxidation of ammonium (N mg liter^{-1})
MERN	fractional maintenance energy requirement for nitrifiers (day^{-1})
NIHP1	rate constant for nitrification inhibitor formation (day^{-1})
NIHP2	rate constant for nitrification inhibitor decay (ml g^{-1} C day^{-1})
NIMX	maximum nitrifier population level (N g m^{-3})
VN	maximum fractional growth rate of nitrifiers (day^{-1})

7. Denitrification

DENP1	maximum rate of denitrification (day^{-1})
DENP2	half-saturation constant for the uptake of nitrate by denitrifiers (N mg liter^{-1})
FDENI	fraction of bacteria which are denitrifiers

8. Mortality

BDRNB	density-dependent death rate for bacteria (day^{-1})
BDRNF	density-dependent death rate for fungi (day^{-1})
BDRTB	maximum death rate due to freezing for bacteria (day^{-1})
BORTF	maximum death rate due to freezing for fungi (day^{-1})
BDRWB	maximum death rate due to drying for bacteria (day^{-1})
BDRWF	maximum death rate due to drying for fungi (day^{-1})
DDD	population density factor limiting mortality (non-dimensional)
ETDBP	effect of soil temperature on bacteria death rate (non-dimensional)
ETDFP	effect of soil temperature on fungi death rate (non-dimensional)
EWDBP	effect of soil moisture on bacteria death rate (non-dimensional)
EWDFP	effect of soil moisture on fungi death rate (non-dimensional)

Driving variables

Driving variables consist of a set of environmental conditions for each of the four soil layers. Driving variables for the present model are supplied by a separate abiotic model (Parton and Singh, 1976; Parton et al., 1978). Driving or decision variables to allow 'management' inputs (i.e., irrigation, fertilization, fumigation, substrate addition) are also included.

1. Abiotic driving variables

TEMPE	average soil layer temperature (°C)
AVMN	average daily air temperature (°C)
AVCM	average daily canopy temperature (°C)
THETA	soil water (fraction)
PRCIP	precipitation (cm day^{-1})

2. Decision variables

FNO3	fertilizer nitrate addition (g m^{-2})
FNH	fertilizer ammonium addition (g m^{-2})
IRRI1	'flag' to initialize soil moisture values following irrigation (non-dimensional)
FUMB	bacterial death due to fumigation (fraction)
FUMF	fungal death due to fumigation (fraction)
CELLU	cellulose addition (C g m^{-2})
GLUCO	glucose addition (C g m^{-2})

10. OBSERVATIONS

Scarcity of complete sets of field data make rigorous validation difficult. Our most reliable field data are for the above-ground portion of grasslands. Some of the validation data available allow only a qualitative evaluation of the model. The most rigorous validations are those involving perturbations. References for the observations and associated experimental designs are given in references in section 11.

11. COMPARISON OF RESULTS

The simulated plant dynamics for one year are shown in Fig. 3. Peak crop for live shoots occurs in August. The precipitous drop in shoot biomass, in October, results from freezing. Peak root biomass occurs after the peak for shoots because the fraction of photosynthate translocated to roots increases throughout the growing season.

Root N concentration decreases during the growing season because carbon is translocated from shoots to roots faster than the plants can take up inorganic N. The increase in root N concentration, during the rest of the year, results from continued N uptake, and from our assumption that dying roots have less N than live roots. Translocation of N to shoots in early April accounts for the dip in root N in April. There is very little data to confirm the predicted dynamics of root biomass and root N content.

Figure 4 gives predicted microbial biomass in the 0 to 2 cm soil layer, which includes

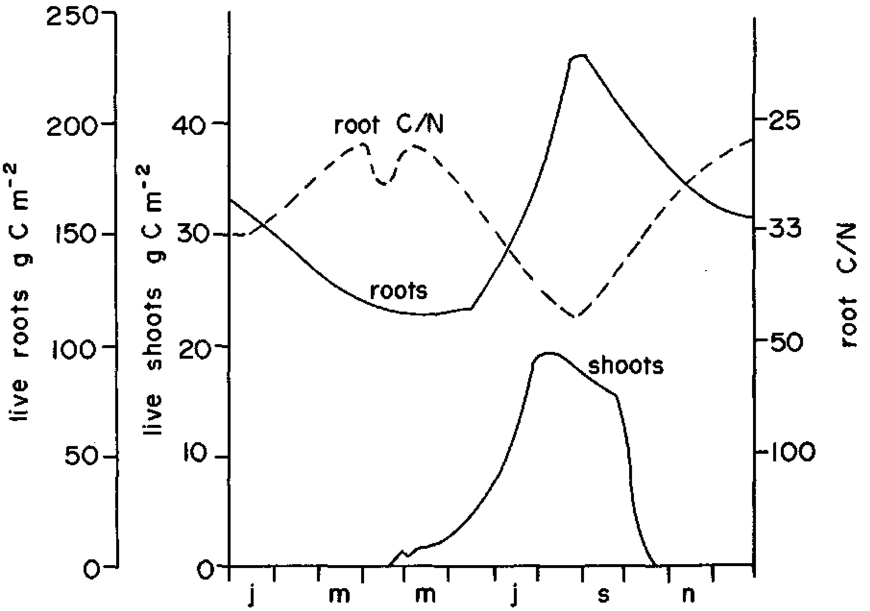


Fig. 3. Predicted shoot and root biomass and root C:N ratio in a blue grama sward during a one-year simulation.

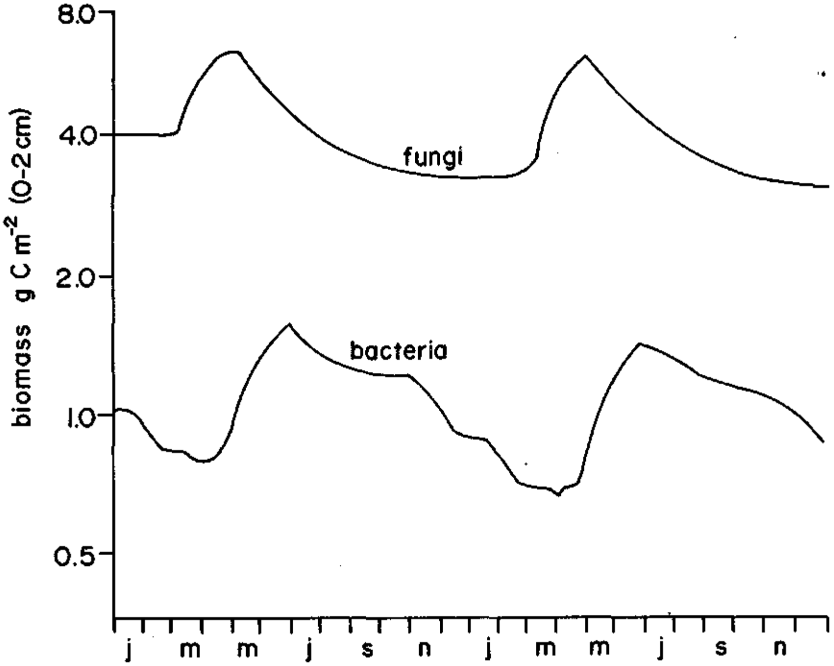


Fig. 4. Predicted microbial biomass in the top two cm over a two-year period.

litter. Fungi are predominant but the model was not 'adjusted' to make fungi dominant. It was adjusted to give total microbial biomass compatible with estimates for grasslands (Woodmansee et al., 1978), but there is little reliable information about the details of microbial dynamics in grasslands. Fungi peak earlier in the year than bacteria, which agrees with the observations reported by Clark and Paul (1970). Microbes are less dynamic than in Hunt's (1977) decomposition model, which distinguished an inactive population from an active fraction with a high growth potential. The presence of a nitrification inhibitor in the model is reflected in low NO_3^- (Fig. 5). There is considerable controversy regarding the presence of a nitrification inhibitor in grasslands. Our intent in this model is only to reflect the possibility of the existence of such compounds. Little or no NO_3^- is formed below 2 cm, where roots are more concentrated and the production of inhibitor is greater. Inorganic N levels decrease dramatically in June - July, when the blue grama is growing fastest.

Most of the C entering the humads component derives from structural litter (Fig. 6) whereas the main supply of N to the humads component is from metabolic litter. Direct transfer of organics to humads from metabolic litter is independent of microbial activity whereas structural litter is transferred to humads as a by-product of decomposition. Only 5.6% of the N leaving the metabolic pool was transferred to humads, the other 94.4% was transferred to microbes.

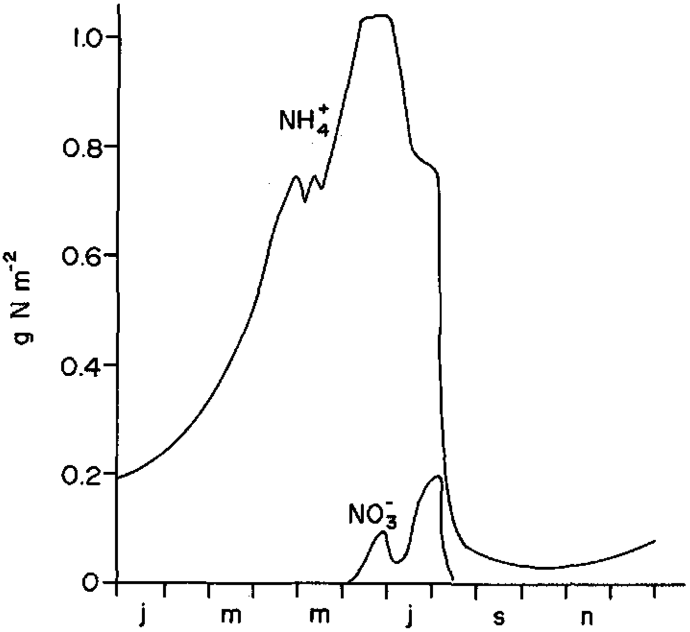


Fig. 5. Predicted inorganic nitrogen in the 0-2 cm layer over a one-year period.

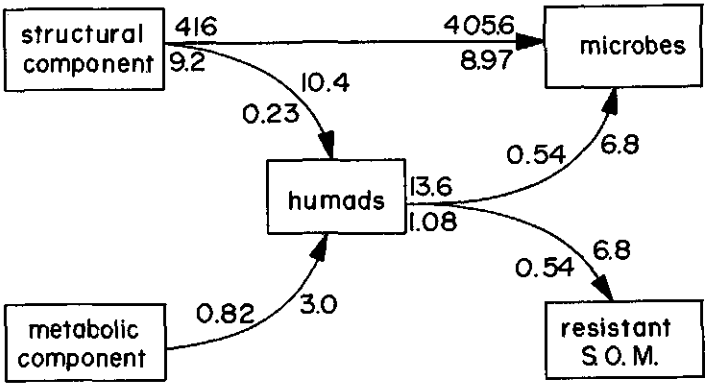


Fig. 6. Simulated rates of formation and decomposition of humads. Carbon fluxes (g C m^{-2} y^{-1}) appear above those of N (g N m^{-2} y^{-1}).

Productivity The model output of 38 g and 44 g C m^{-2} maximum standing crop in the first and second years, respectively, compares favorably with field observations at the Pawnee Site, although the model was not tuned to a set of field data. Observed standing crops during the actively growing season averaged 43 g C m^{-2} and ranged between 30 and 55 g C m^{-2} (Clark, 1977) for individual blue grama patches. Maximum live standing crop was 30 g C m^{-2} in 1974 and about 40 g C m^{-2} in 1975 (Parton et al., 1978). Dodd and Lauenroth (1979) reported total aboveground production of 100 g dry ash free biomass m^{-2} in 1973, which can be converted to 45 to 50 g C m^{-2}. Our simulated value for aboveground production in 1973 is 50 g C m^{-2}.

Respiration Independent field measurements of soil respiration have been made but they are infrequent and are not available for 1973, the year of the simulation. Evolution of CO_2 in other years is variable in the field and in the simulation runs. Simulated rates generally fall within the range of measured values but tend to be lower than average. Rates of CO_2 evolution, from roots and microbes in the model, show less response to moistening and drying than did respiration in the Hunt (1977) model.

Cumulative simulated total output of CO_2-C/year of 286 g C m^{-2} with 24% of the total respired by roots compares with the estimates of Coleman et al. (1976) who calculated 276 g C m^{-2} based on field measurements and corrections for temperature and moisture fluctuations.

Top:Root ratios Grasslands normally have higher root than live top biomass. Sims et al. (1978) reported a root:shoot ratio of 10:1 for the arid grasslands modeled here. Their measurements included all root materials, many of which may have been dead. Woodmansee et al. (1978) calculated a live root:shoot ratio of 4:1 for the Pawnee Site. Our model at peak standing crop predicts ratios of 6.1:1 and 5.6:1 for the two years, which were closer to those of Woodmansee et al. (1978) than to those of Sims et al. (1978) Early and late in the growing season the ratio of live roots:shoots according to the model was greater than at peak crop. Field measurements would be expected to vary considerably over a growing season.

Mineral N content of soil The mineral N level in dried soil samples on July 29, 1973 totalled 1.9 and 0.1 g N m^{-2} as NH_4^+ and NO_3^-, respectively (Woodmansee et al., 1978). The simulated values for that day (0.27 and 0.03 g N m^{-2} as NH_4^+ and NO_3^-, respectively) are lower than those measured. This is not a serious problem for two reasons: (a) the data for which information is available is when plant growth is causing a rapid depletion in the soil mineral N; and (b) NH_4^+ was likely released upon drying. The model predicts mineral N levels similar to those measured but about two weeks earlier. This may correspond to the lag of about one week between dates of observed and simulated peak standing crop.

Turnover of microbes Turnover rate of microbial C can be calculated from the model output. It is taken as Death (C)/Biomass (C) for each microbial group. The microbial population turned over an average of 5.5 times. Fungal activity dominated with 7.7 generations while only 80% of the bacterial population regenerated in one year. Clark and Paul (1970) concluded that the soil microbial population could reproduce only about 4.5 times per year.

The model is consistent with their estimate but also suggests most of the activity is fungal.

12. LIMITS AND LIMITATIONS

The model emphasizes the biological and biochemical soil-plant subsystem including plants, microbes, organic residues and mineral N. Temperature and moisture are driving variables. Less dynamic state variables such as soil pH, cation exchange capacity, texture, mineralogy, and structure are not included explicitly; nor are soil animals.

The most mechanistic process treatments include nitrification, root uptake of inorganic N, mineralization, immobilization, and humification. Treatments of plant growth, phenology, plant response to N, and N redistribution during growth and senescence are treated sufficiently mechanistically that the primary producer submodel can provide substrates to and interact with the decomposition portion of the model. The treatments of denitrification and leaching are simplistic, and biological di-nitrogen fixation is included with a general atmospheric input function. Ammonia volatilization is not included, nor is non-exchangeable NH_4^+ fixation by clays.

Development of the model has shown a scarcity of information in the literature about several processes. Among these are the mechanisms by which environmental factors affect microbial and plant growth, activity, and death in soil, and the fate of N in plant roots upon their death in soil. No good treatment of NH_4^+ diffusion to nitrifiers exists and no good way has been reported to treat O_2 supply and microsite spatial variability, which is essential to understanding denitrification. Information is needed on trophic interactions in soil and good quick methods to measure live and active biomass of specific taxa are still lacking. There is still a lack of quantitative information about physical protection of organics in soil. Ways to separate soil organic components into groups relating to biological availability in soil await further improvement. At present the greatest overall need is for data and concepts relating to control mechanisms in soil at the microsite level, and for appropriate validation data. These questions have been dealt with at length by Van Veen et al. (1980).

13. COMPUTER

Control Data Corporation Cyber 170 Series.

14. LANGUAGE

SIMCOMP 4.0, a FORTRAN-based simulation language developed at Colorado State University. We are converting PHOENIX to a new simulation package recently developed at the Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado, USA. The new package provides the same support as SIMCOMP 4.0 along with enhanced output capabilities. The simulation package allows models to be written in standard FORTRAN and the simulation software has been designed to be as machine-independent as possible. The software package is operational on CDC Cyber 170 and PDP 11 Series machines and will soon be implemented on IBM 360 Series hardware. Other models of a similar size to PHOENIX have shown a substantial time/cost savings when converted from SIMCOMP to the new system. Overall run time/cost, including compilation, has been about 40 percent of that using SIMCOMP. Model conversion is scheduled for completion by July, 1980.

15. RUN TIME/COST

For a two-year simulation run, present compilation time takes 70 CPU seconds and execution time takes 300 CPU seconds at an approximate cost of $6.00/minute of CPU time. See also section 14.

16. USERS

PHOENIX is currently being used to support research at Colorado State University, The University of Alberta, Edmonton, Canada, and the Swedish University of Agricultural Sciences, Uppsala, Sweden. A version in which the time step for bacterial and fungal growth has been converted to one day has replaced the decomposition (Hunt, 1977) and nitrogen (Reuss and Innis, 1977) submodels of the grassland ecosystem model (ELM) at the Natural Resource Ecology Laboratory (Innis, 1978). The revised grassland ecosystem model (GEM) is currently being used in several ecosystem level research projects.

17. DEVELOPER AND PRINCIPAL CONTACT

The authors of this paper are the developers of the model.

REFERENCES

Clark, F.E., 1977. Internal cycling of ^{15}nitrogen in shortgrass prairie. Ecology 58: 1322-1333.

Clark, F.E., & E.A. Paul, 1970. The microflora of grassland. Advances in Agronomy 22: 375-435.

Coleman, D.C., R. Andrews, J.E. Ellis, & J.S. Singh, 1976. Energy flow and partitioning in selected man-managed and natural ecosystems. Agro-Ecosystems 3: 45-54.

Dodd, J.L., & W.K. Lauenroth, 1979. Analysis of the response of a grassland ecosystem to stress. In: N.R. French (Ed): Perspectives in grassland ecology. Springer-Verlag, New York, p. 43-58.

Hunt, H.W., 1977. A simulation model for decomposition in grasslands. Ecology 58. 469-484.

Innis, G.S., 1978. Grassland simulation model. Ecological Studies, Vol. 26. Springer-Verlag, New York.

Parton, W.J., & J.W. Singh, 1976. Simulation of plant biomass on a shortgrass and a tallgrass prairie with emphasis on below-ground processes. US/IBP Grassland Biome Tech. Rep. No. 300. Colorado State University, Fort Collins, 76 p.

Parton, W.J., J.S. Singh, & D.C. Coleman, 1978. A model of production and turnover of roots in shortgrass prairie. Journal of Applied Ecology 47: 515-542.

Reuss, J.O., & G.S. Innis, 1977. A grassland nitrogen flow simulation model. Ecology 58: 379-388.

Sims, P.L., J.S. Singh, & W.K. Lauenroth, 1978. The structure and function of ten western

North American grasslands. I. Abiotic and vegetational characteristics. Journal of Ecology 66: 251-285.

Van Veen, J.A., W.B. McGill, H.W. Hunt, M.J. Frissel, & C.V. Cole, 1980. Simulation models of the terrestrial nitrogen cycle. In: F.E. Clark & T. Rosswall (Eds): Terrestrial nitrogen cycles: Processes, ecosystem strategies, and management impacts. Ecological Bulletins (Stockholm) (in press).

Woodmansee, R.G., J.L. Dodd, R.A. Bowman, F.E. Clark, & C.E. Dickinson, 1978. Nitrogen budget of a shortgrass prairie ecosystem. Oecologia (Berl.) 34: 363-376.

4.10 PAPRAN: A simulation model of annual pasture production limited by rainfall and nitrogen

N.G. Seligman and H. van Keulen

1. NAME

PAPRAN: Production of arid pastures limited by rainfall and nitrogen.

2. SYSTEM MODELED

The model is applicable to a field of annual pasture or a small-grain crop growing in a homogeneous soil in a semi-arid environment.

3. OBJECTIVE

PAPRAN has a dual objective:

a. *Applied* To determine the biological and economic efficiencies of different crop and pasture management systems in the fluctuating and uncertain climatic environment of semi-arid regions. In particular, the purpose is to generate data that are difficult to obtain by other means, e.g. data for a series of years long enough to characterize a region or data that involve complex measurement techniques and high costs even in a single year. It is envisaged that it will be used to analyze different fertilization and grazing management options for arid zone agropastoral systems.

As both water and nitrogen availability are among the major determinants of crop yield and pasture productivity in the semi-arid zone, PAPRAN concentrates on these factors and on the inter-relations between them.

b. *Scientific* To test hypotheses relating to the water and nitrogen balance, plant growth, seed production, grazing effects and secondary production in semi-arid environments. In particular - hypotheses on the relative importance of water and nitrogen under fluctuating climatic conditions; on the inter-relations between nitrogen and water supply on the one hand, and dry matter and nitrogen distribution between seeds and other components of the plant biomass on the other hand. The purpose is to identify and quantify those processes which are particularly important in determining crop and pasture growth where moisture and nitrogen are limiting so that research, both field and more fundamental, can be directed towards improved understanding in these areas.

4. TIME SCALE

Basically PAPRAN models one growing season (generally less than seven months between germination and maturity) with a time resolution of one day.

5. STRUCTURE OF THE MODEL

The main elements of the structure of PAPRAN are illustrated in a simplified relational diagram (Fig. 1). They include compartments that represent the biomass and nitrogen content of an annual crop or pasture canopy, the soil (organic matter, nitrogen and water) and the environmental variables.

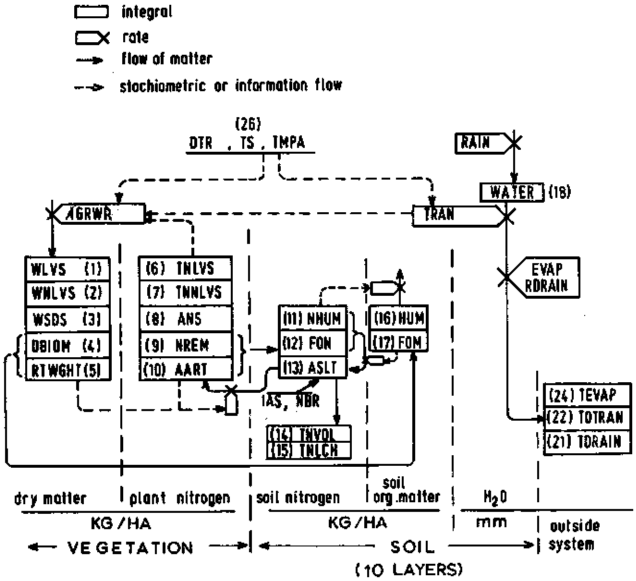


Fig. 1. A simplified relational diagram of the simulation model PAPRAN (for the explanation of symbols, see sections 6, 7, 8).

6. LEVELS

The plant dry matter is divided into (kg ha^{-1}, d.m):

1.	WLVS	leaves
2.	WNLVS	non-leaf vegetative material
3.	WSDS	seeds
4.	DBIOM	dead plant material
5.	RTWGHT	roots

Nitrogen in each of the vegetation compartments is defined as follows (kg ha^{-1}, N):

6.	TNLVS	nitrogen in leaves

7.	TNNLVS	nitrogen in non-leaf material
8.	ANS	nitrogen in seeds
9.	NREM	nitrogen in dead plant material
10.	AART	nitrogen in roots

The soil profile is divided into ten layers with variable thickness, THCKN$_i$. The number and thickness of the layers can easily be changed. Soil nitrogen in each compartment is divided into (kg ha^{-1}, N):

11.	NHUM$_i$	nitrogen in stable organic material ('humus')
12.	FON$_i$	nitrogen in fresh organic material
13.	ASLT$_i$	mineral nitrogen, expressed as nitrate

Nitrogen lost from the system is totalized in the following integrals (kg ha^{-1}, N):

14.	TNVOL	nitrogen lost by volatilization
15.	TNLCH	nitrogen lost by leaching

The organic matter fraction of each soil layer is divided into two (kg ha^{-1}, d.m):

16.	HUM$_i$	stable organic material
17.	FOM$_i$	fresh organic material

Soil moisture is monitored in each layer (mm, H_2O)

18.	WATER$_i$	soil moisture

The other elements of the water balance are totalized (in mm, H_2O) in the following integrals:

19.	TRAIN	rainfall
20.	TOTINF	infiltration (runoff can be taken into account)
21.	TDRAIN	drainage
22.	TOTRAN	transpiration from vegetation
23.	PPEVAP	potential evapo-transpiration
24.	TEVAP	evaporation from bare soil surface

Some auxiliary variables are also defined as integrals:

25.	CTRDEF	cumulative relative transpiration deficit (-)
26.	TS	soil temperature, 10-day running average of air temperature for total soil profile (^{o}C)
27.	TMPSUM	temperature sum from germination (day x ^{o}C)
28.	AMAX	maximum assimilation rate (kg ha^{-1} (leaf area) h^{-1}, CO_2)
29.	EFFE	photosynthetic efficiency (kg ha^{-1} h^{-1})/J m^{-2} s^{-1})
30.	LFAREA	leaf area (m^{2} ha^{-1})
31.	SLCVR	effective soil cover by vegetation (m^{2} ha^{-1})
32.	DVS	development stage of vegetation (-)

33. RTD rooting depth (mm)

34. RANO3 relative amount of nitrate in top soil layers (-)

7. GOVERNING EQUATIONS

The conceptual basis of PAPRAN

Conceptually, PAPRAN is a soil-water balance model where plant growth is closely related to water transpired and to the nitrogen status of the vegetation. The soil water balance and the plant growth sections are developed as in ARID CROP (Van Keulen, 1975; Van Keulen et al., 1980); the nitrogen uptake and redistribution in the plant is based on a relatively simple representation of these processes as supply and demand balances (Seligman et al., 1975); the nitrogen cycling between plant and soil as well as the nitrogen transformations in the soil are represented as immobilization and mineralization processes dependent on environmental factors and on the C:N ratio of the organic material (Beek and Frissel, 1973; Parnas, 1975).

The resolution of PAPRAN is determined largely by its objective: it is meant to simulate plant canopy growth in field conditions relevant to crop and pasture management. Thus, the boundary conditions as well as the plant, soil and environmental parameters for specific situations must be available or measurable by standard procedures. This means that many of the processes cannot be realistically described as basic physical, chemical or microbiological reactions, but have to be mimicked, i.e. they have to be stated as essentially black box transformations. Consequently, generality is reduced and the application of the model is limited to situations which do not differ widely from those that have been used for validation (or, in other words, those for which the model has been calibrated).

Processes

The processes that define the relationships between the state variables and their rates of change are divided into the following sections:

A. plant growth,

B. nitrogen uptake by the plant,

C. soil organic matter and nitrogen transformations,

D. soil water balance.

A. *Plant growth*

This section has been described in detail elsewhere (Van Keulen, 1975; Van Keulen et al., 1980), so only the central concepts and processes will be recapitulated here.

Daily dry matter production: The calculation of plant growth (= total dry matter production) unrestricted by nitrogen shortage, is based on the fact there is a close relationship between water use and plant growth when water is limiting and plant nutrients are not (De Wit, 1958). The assumption applied in this model is that nitrogen deficiency in the plant tissue reduces the growth rate without affecting plant water use. There are indications that this assumption does not hold under all conditions (Goudriaan and Van Keulen, 1979). The central equation is:

$$\mathrm{AGRWR} = \mathrm{TRAN} * \mathrm{WUSEFF} * \mathrm{REDFNS} \tag{1}$$

where

AGRWR = actual total daily dry matter production (kg ha^{-1} day^{-1})
TRAN = daily transpiration by canopy (mm day^{-1})
WUSEFF = water use efficiency (kg ha^{-1} mm^{-1})
REDFNS = reduction factor for nitrogen deficiency (-).

$$\mathrm{TRAN} = f(\mathrm{APTRAN}, \mathrm{RTL}_i, \mathrm{WATER}_i, \mathrm{TEC}, \mathrm{CONC}_i) \tag{2}$$

$$\mathrm{APTRAN} = \mathrm{PTRAN} * \mathrm{RFDVS} \tag{3}$$

$$\mathrm{RFDVS} = f(\mathrm{DVS}) \tag{4}$$

$$\mathrm{PTRAN} = f(\mathrm{VPA}, \mathrm{MXT}, \mathrm{MNT}, \mathrm{WSR}, \mathrm{DTR}, \mathrm{LFOV}, \mathrm{DAYL}) \tag{5}$$

where

PTRAN = potential daily transpiration rate (mm day^{-1}); calculated on the basis of the Penman equation (Penman, 1948)
VPA = vapour pressure of the air (mm Hg)
MXT, MNT = maximum and minimum air temperature ($^{\circ}$C)
WSR = wind-run (km day^{-1})
DTR = daily total global radiation (cal cm^{-2} day^{-1})
LFOV = fraction of sky that is overcast (-)
DAYL = day length (h)
DVS = development stage of the vegetation, dependent on accumulated temperature
RFDVS = reduction factor for potential transpiration which is reduced as the plants approach maturity
RTL_i = depth of root penetration in each soil layer (mm)
TEC = factor that relates root conductivity to soil temperature (-)
CONC_i = salt (= nitrate) concentration, reducing transpiration rate at high values.

$$\mathrm{WUSEFF} = \mathrm{PDTGR}/\mathrm{PTRAN} \tag{6}$$

$$\mathrm{PDTGR} = (\mathrm{PDTGAS}-\mathrm{MAINT}) * \mathrm{CONFS} \tag{7}$$

$$\mathrm{PDTGAS} = f(\mathrm{DAYY}, \mathrm{LAT}, \mathrm{LFOV}, \mathrm{LAI}, \mathrm{AMAX}, \mathrm{EFFE}) \tag{8}$$

MAINT = TDRWT * MRESF * TEFR (9)

where

PDTGR = potential daily growth rate (kg ha^{-1} day^{-1}, dry matter)
PDTGAS = potential daily gross assimilation rate (kg ha^{-1} day^{-1}, CH_2O). Calculated with an algorithm developed by Goudriaan and Van Laar (1978).
MAINT = maintenance respiration (kg ha^{-1} day^{-1}, CH_2O)
CONFS = conversion efficiency by weight from carbohydrate to structural plant material
DAYY = calendar day (Julian day)
LAT = latitude (degrees)
LAI = leaf area index (-)
AMAX, EFFE = see section 5. In PAPRAN, both AMAX and EFFE can be reduced by water stress due to prolonged drought; they can also recover after termination of the drought.
TDRWT = total dry weight of live plant material, including roots (kg ha^{-1}, d.m.)
MRESF = maintenance respiration requirement (kg (CH_2O) kg^{-1} (d.m) day^{-1})
TEFR = temperature effect on maintenance respiration ($Q_{10} = 2$).

$$REDFNS = 1.-\sqrt{(1-y^2)} \qquad (10)$$

$$Y = (FNLVS-LN)/(MNGLV-LN),\ 0 \leq Y \leq 1 \qquad (11)$$

where

FNLVS = nitrogen concentration in leaves (kg (N) kg^{-1} (d.m.))
MNGLV = leaf nitrogen concentration threshold for unrestricted growth (kg (N) kg^{-1} (d.m.)), function of DVS. The value declines as the plants age.
LN = leaf nitrogen concentration threshold below which there is no growth (kg (N) kg^{-1} (d.m.)).

The reduction function is taken from Seligman et al. (1975) and is based on a qualitative description of the process as suitable experimental data were not found.

Allocation of dry matter: The daily increment in dry matter is allocated to growth of different plant parts: first, shoots and roots; then shoot growth is sub-divided into leaf, non-leaf vegetative material and seeds. The allocation is governed by the development stage of the vegetation, DVS.

GROWTR = AGRWR * CSRR (12)

CSRR = f(DVS, FAMST) (13)

where

GROWTR = growth rate of shoot (kg ha^{-1} day^{-1}, d.m.)
CSRR = current shoot to root ratio (dimensionless); the amount of dry matter invested in the roots decreases as the vegetation matures
FAMST = factor that reduces shoot allocation as water stress increases; dependent on the relative transpiration deficit, RTRDEF (= (APTRAN - TRAN)/APTRAN).

$$GROWTV = GROWTR * (1-FRTS) \quad (14)$$

$$GRLVS = GROWTV * DISTF \quad (15)$$

where

GROWTV = growth rate of vegetative parts (kg ha^{-1} day^{-1}, d.m.)
GRLVS = growth rate of leaves (kg ha^{-1} day^{-1}, d.m.)
FRTS = fraction of dry matter allocated to seeds, dependent on DVS
DISTF = fraction of vegetative growth allocated to leaves; dependent on DVS and FANS. The latter governs the influence of nitrogen stress on the partitioning of dry matter between leaves and stems. FANS drops from 1 to 0.5 as the fraction of nitrogen in the leaves, FNLVS, drops below the threshold for unrestricted growth of leaves, MNGLV, to the limiting nitrogen concentration for growth, LN.

The allocation of dry matter to seeds and non-leaf vegetative parts is thus GROWTR * FRTS and GROWTV * (1-DISTF), respectively.

Death of vegetative tissue: Vegetative material can die as a result of stress due to water or nitrogen deficiency or due to natural death of maturing annual plants as development is completed or the season ends. The death rate of leaves, RDLVS, and of non-leaf material, RDNLVS is calculated as follows:

$$RDLVS = \begin{cases} RDLVS1, & PCTRAN > TRAN \\ RDLVS2, & \text{otherwise} \end{cases} \quad (16)$$

where

PCTRAN = potential cuticular transpiration, assuming fully closed stomata; calculated by substituting cuticular resistance, RC, for stomatal resistance, RS, in the calculation of PTRAN. RC is assumed to be 20 * RS.

$$RDLVS1 = RDLVSX/TCDRL \quad (17)$$

where

RDLVSX = amount of dry matter in leaves that would have to be dehydrated in one day to make up the difference between PCTRAN and TRAN

TCDRL = time constant that represents the buffering capacity of the leaf tissue to dehydration. In PAPRAN, the time constant is taken as 5 days. Both TCDRL and RC need to be verified experimentally, even though the present values simulate actual drying situations reasonably well (Van Keulen et al., 1980).

$$RDLVS2 = AMAX1\ (RDRD,\ RDRN) * WLVS \qquad (18)$$

where

RDRD = death rate due to senescence, - 0 when DVS < 0.7 then rises to 0.005 and when DVS > 0.9 it rises to 0.1

AMAX1 = a function, which takes as output the maximum value of its argument.

$$RDRN = 0.3 * \left(1 - \sqrt{1 - (1-Y)^2}\right) \qquad (19)$$

Y - see Eqn. (11).

Rate of dying of non-leaf material, RDNLVS, is, in principle, calculated identically to RDLVS, so that

$$RDNLVS = RDLVS * WNLVS/WLVS \qquad (20)$$

B. *Nitrogen uptake*

It is assumed that nitrogen is taken up as nitrate and that the root system of the canopy is dense and efficient down to the whole rooted depth (Van Keulen et al., 1975). Consequently, nitrate is highly available to the plant, either by mass transport with the transpiration stream or by diffusion of anions along a concentration gradient created by low nitrate concentration at the root surface. Thus, the nitrogen demand of the plant can be satisfied within a relatively short time. From experimental studies, it appears that a time constant of about two days is reasonable (Dijkshoorn et al., 1968).

The demand for nitrogen is created by the difference between the current nitrogen content of the plant and an optimum content. The latter decreases as the development of the plant proceeds. The present version of the model assumes that under limited nitrogen supply, the actual amount of nitrogen taken up is divided between shoot and root in proportion to their relative demands (Van Dobben, 1961). Seed demand for nitrogen is met by the vegetative parts of the plant, thus increasing the demand of nitrogen from the soil. As tissues become depleted, translocation to the seeds becomes retarded and the demand for nitrogen in the seed is not met, resulting in seed with a lower nitrogen content.

These processes are defined as follows:

Uptake:

$$RNU = TNUM + TNUDF \tag{21}$$

where

RNU = rate of nitrogen uptake (kg ha^{-1} day^{-1}, N)
TNUM = nitrogen uptake from the rooted depth by mass flow, $\sum_i RNUM_i$, dependent on concentration of nitrogen in the soil, $CONC_i$, and the transpiration stream, TRR_i, from each soil layer
TNUDF = nitrogen uptake by diffusion from the rooted depth.

$$TNUDF = \sum_i (AMIN1\ (RNUD_i,\ ASLT_i/DELT-RNUM_i-RNAC_i)) \tag{22}$$

$$RNUD_i = RNUDF * \sum_i (ASLT_i-RNAC * DELT)/TNRT) * (RTL_i/THCKN_i)) \tag{23}$$

$$RNUDF = (PNUDP - TNUM) \tag{24}$$

$$PNUDP = AMIN1\ (NDEM,\ TNRT/DELT,\ MUPTR) \tag{25}$$

$$MUPTR = MNU * (1 - e^{-.5 * TVEGM/CF})$$

where

$RNUD_i$ = rate of uptake by diffusion (kg ha^{-1} day^{-1}, N), effective only when moisture content in layer i is above wilting point
$RNUM_i$ = uptake rate by mass flow from each soil layer (kg ha^{-1} day^{-1}, N)
$RNAC_i$ = rate of immobilization of nitrogen by decomposers (kg ha^{-1} day^{-1}, N)
RNUDF = required rate of uptake of inorganic N by diffusion from the rooted depth (kg ha^{-1} day^{-1}, N)
TNRT = total inorganic N in those layers where both roots and available moisture are present (kg ha^{-1}, N)
PNUDP = daily inorganic N uptake potential (kg ha^{-1} day^{-1}, N)
DELT = time interval of integration (= 1 day)
TAU2 = time constant (= 2 days)
NDEM = nitrogen demand of the vegetation (kg ha^{-1} day^{-1}, N)
MUPTR = maximum uptake rate of canopy (kg ha^{-1} day^{-1}, N)
MNU = maximum uptake rate of closed canopy (= 9 kg ha^{-1} day^{-1}, N)
TVEGM = weight of vegetative mass, WLVS + WNLVS (kg ha^{-1}, d.m.)
CF = weight/area coefficient of vegetative mass (kg ha^{-1}). MUPTR represents the transfer tissue necessary to take up nitrogen, related to the vegetation cover here, as a function of TVEGM/CF. A similar function has been used (Van Keulen,

1975), to represent relative vegetation cover of the soil. Here it is assumed, that the tissue is proportional to the lateral extension of the roots, which is probably greater than the vegetation cover; thus a lower value for CF is used.

Demand:

$$NDEM = (SDEM + NDRT) * EOSF \tag{26}$$

$$EOSF = \begin{cases} 1., & DVS < 1 \\ 0, & \text{otherwise} \end{cases} \tag{27}$$

$$NDRT = (RTWGHT * MFRT - AART)/TAU2 \tag{28}$$

$$SDEM = NDLVS + NDNLVS \tag{29}$$

$$NDLVS = (WLVS * MXNLV - TNLVS)/TAU2 \tag{30}$$

$$NDNLVS = (WNLVS * MXNNLV - TNNLVS)/TAU2 \tag{31}$$

SDEM = nitrogen demand of the shoot (kg ha^{-1} day^{-1}, N)

where

EOSF = factor to prevent uptake after maturity
NDRT, NDLVS, NDNLVS = nitrogen demand of the root, the leaves and the non-leaf material, respectively (kg ha^{-1} day^{-1}, N)
MFRT, MXNLV, MXNNLV = optimum level of nitrogen in roots, leaves and non-leaf material, respectively, dependent on DVS (kg (N) kg^{-1} (d.m.))

Allocation:

$$RNUS = RNU * SDEM/(SDEM + NDRT) \tag{32}$$

$$RNULV = RNUS * NDLVS/SDEM \tag{33}$$

$$RNUNLV = RNUS * NDNLVS/SDEM \tag{34}$$

$$RNURT = RNU * NDRT/(SDEM + NDRT) \tag{35}$$

$$RNS = WSDS * (ONC - FNS) * RFNS/TAU2 \tag{36}$$

$$RFNS = 1 - 1-Y^2 \qquad (37)$$

where

RNUS, RNULV, RNUNLV, RNURT, RNS = rate of nitrogen flow to shoot, leaves, non-leaf material, root and seeds, respectively (kg ha^{-1} day^{-1}, N)

ONC = optimum concentration of nitrogen in the seeds, dependent on development stage in the reproductive phase. ONC drops from the nitrogen concentration of young tissue (0.045) to the nitrogen concentration of mature seeds optimally supplied with nitrogen. This, too, is species dependent and is taken as 0.025 for cereals and grasses.

FNS = fraction of nitrogen in the seeds (kg (N) kg^{-1} (d.m.))

RFNS = reduction factor on nitrogen flow to seeds due to nitrogen deficiency in the leaves; implies that flow is severely reduced when nitrogen concentration in the leaves falls below the optimum for unrestricted growth.

Translocation: In PAPRAN, nitrogen supply to the seeds comes from the nitrogen in the vegetative material and not directly from the roots. In reality this may not be strictly true, but even with an integration step of one day the demand will be transferred to the vegetative tissue and from there to the roots within a short time. The nitrogen is withdrawn from leaf and non-leaf material in proportion to the amounts of nitrogen in each of them.

Nitrogen in the above-ground live vegetative material is also withdrawn by dying leaves, RNLD, and non-leaf material, RNLDN. The concentration of nitrogen in the dying tissue depends on the cause of death: if the tissue dies because of water shortage or senescence, the dead tissue nitrogen concentration is the same as that in the live tissue, FNLVS, or FNNLVS; if the reason is nitrogen deficiency, the nitrogen concentration is the unextractable residual, LN. This is expressed as follows:

$$RNLD = RDLVS * \begin{cases} FNLVS, & PCTRAN > TRAN \text{ or } RDRD > RDRN \\ LN, & \text{otherwise} \end{cases} \qquad (38)$$

The rate of nitrogen loss from live non-leaf material, RNLDN, is calculated in the same way, substituting RDNLVS and FNNLVS for RDLVS and FNLVS.

C. *Soil organic matter and soil nitrogen transformations*

a. Conceptual background:

The complexity and importance of soil nitrogen transformations has given rise to a voluminous literature (Bartholomew and Clark, 1965; Tandon, 1974; Van Veen, 1977). This can be used to design detailed models of the soil nitrogen system (e.g. Beek and Frissel, 1973; Hagin and Amberger, 1974; Van Veen, 1977). Van Veen (1977) has demonstrated that it is useful to divide the overall model into sub-models that deal with the main states and processes separately but still influence each other through the relevant state variables. In such model the microbial biomass and its associated nitrogen are considered as separate pools. However, because of serious methodological limitations (Van Veen, 1977) it is difficult to initialize the microbial biomass values (and even the easier-to-measure soil organic matter components) for specific field situations. Also, in many crop growth models, only a few of the nitrogen states are of direct interest and the complexity of a general model is sure to add a great deal of spurious detail. In order to include a soil nitrogen section in PAPRAN compatible with the time-resolution of the other parts of the model, soil nitrogen was lumped into three states only, - mineral nitrogen (including NH_4^+, NO_2^-, NO_3^-); nitrogen in fresh organic material (including nitrogen in plant residues and in the microbial biomass); and nitrogen in the 'stable' organic fraction, or the humus fraction. Thus microbial biomass is not treated separately but is assumed to be part of the fresh organic material. Consequently microbial nitrogen is part of the fresh organic nitrogen pool.

This approach necessitates lumping some of the processes and their associated parameters:

- immobilization becomes total immobilization of all mineral nitrogen by the microbial growth. The rationale for this simplification is based on the fact, that the microbial population of soil, responsible for decomposition, is highly diverse and can easily adapt itself to the source of mineral nitrogen.
- mineralization of nitrogen to NH_4^+ and nitrification to NO_3^- are treated as one transformation. The justification for so sweeping a generalization is based on the fact that in well areated semi-arid soils the transformation $NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$ is normally not inhibited by environmental conditions, or by lack of suitable oxidizing micro-organisms. Soon after the microbial population is activated, the transformations proceed rapidly, so that there is, in fact, practically no accumulation of NH_4^+ or of NO_2^- (Van Veen, 1977). The limiting process is generally the decomposition rate of the fresh organic matter. That is not always true as recent experimental evidence from the Sahel (Krul, 1980) has shown that ammonium may accumulate, especially after hot, dry periods, when there is apparently a depletion of nitrifying organisms. This could possibly be caused by partial soil sterilization as soil surface temperatures rise above 50 °C (Russell, 1958). Such situations are clearly not covered by PAPRAN, because not only would it be necessary to separate the mineral nitrogen into its NH_4^+ and NO_3^- fractions, but the nitrifying micro-organisms would have to be treated separately from the fresh organic matter decomposers - each with their own different responses to environmental factors.

Lumping microbial biomass with fresh organic material presents problems, e.g.:

a. how to deal with the lag caused by initial build up and subsequent adaptations of microbial populations,

b. how to deal with the effect of dead microbial biomass on the composition of the fresh organic material.

With seasonal crop growth models, the first problem can generally be neglected (especially in non-extreme situations), as the adaptation rate of the microbial population to major changes in substrate is of the order of days (Van Veen, 1977). As a result initial number of micro-organisms per se will not seriously limit decomposition on a seasonal basis. The controlling factors will then be temperature, moisture and available carbon and nitrogen substrate. In PAPRAN the C:N ratio is used to reduce the decomposition rate of fresh organic matter when the C:N ratio exceeds 25. The available mineral nitrogen is taken into account by including it in the calculation of the current C:N ratio of the decomposition system. This approach is based on Parnas (1975).

The second problem is part of a wider one as the decomposition rate constant depends on the composition of the fresh organic material. This is taken into account by changing the rate constant sequentially as the more easily decomposable fractions of the fresh organic material vanish. The switch for changing the rate constant can be adjusted according to the composition of the fresh organic material in question. As PAPRAN considers mainly the re-cycling of natural plant residues with fairly constant composition, the swithching function has been regarded as a constant too. It has been shown that when the soil is rewetted after a hot, dry period, there is a flush of mineralisation. This is possibly due to decomposition of microbial biomass, killed by partial sterilization before wetting. Thus the composition of the lumped fresh organic matter can fluctuate during the growing season. This process could be treated within the general resolution of PAPRAN, but has not yet been incorporated.

- Volatilization of NH_4^+ from the top soil layer is dependent on the ammonia concentration, on pH and on temperature (Van Veen, 1977). pH is not simulated in PAPRAN, and so must be regarded as constant. As the time constants of the chemical processes involved are much smaller than the resolution of PAPRAN, volatilization is approximated by a mimicking procedure. This can be inaccurate when nitrogen fertilizer given as urea or ammonium sulphate is applied to the surface of a pasture sward without thorough incorporation into the soil.
- Adsorption of NH_4^+ to the exchange complex is disregarded because it is a relatively constant fraction of the soil N and can have only a small effect on the seasonal nitrogen balance. Fixation of NH_4^+ into the clay mineral lattice is neglected as it is not significant in most soils of interest in the arid zone (Feigin and Yaalon, 1974). Fertilizer nitrogen is regarded as nitrate, on the assumption that applied ammonia is converted to nitrate much more rapidly than the early season germinating vegetation can take it up.

b. Soil organic matter transformations:

For each relevant soil layer, two organic components are defined:

FOM_i fresh organic material, which includes roots of the previous year and other plant and microbial residues (kg ha^{-1}, d.m.)

HUM_i stable organic material (kg ha^{-1}, d.m.)

The decomposition rate of the fresh organic material is based on first-order kinetics, modified by factors for moisture, temperature and the C:N ratio, where the available mineral nitrogen is included in its calculation. The rate constant depends on the composition of the organic material. Beek and Frissel (1973), give the following values in day^{-1}:

sugars and proteins = 0.08; celluloses and hemi-celluloses = 0.005; lignin = 0.00095. These are however, clearly too low by an order of magnitude (Hagin and Amberger, 1974; Jansson, 1958).

In PAPRAN the rate is changed in a step-wise manner as the original amount of fresh organic material is reduced.

The equations are as follows:

$$\mathrm{DECR}_i = \mathrm{FOM}_i * \mathrm{RDECR}_i * \mathrm{TF} * \mathrm{CNRF}_i * \mathrm{MF}_i \tag{39}$$

$$\mathrm{RDECR}_i = \begin{cases} \mathrm{RDCARB},\ \mathrm{FOM}_i/\mathrm{IFOM}_i > 0.8 \\ \mathrm{RDCELL},\ 0.1 < \mathrm{FOM}_i/\mathrm{IFOM}_i < 0.8 \\ \mathrm{RDLIGN},\ \mathrm{FOM}_i/\mathrm{IFOM}_i < 0.1 \end{cases} \tag{40}$$

RDCARB, RDCELL, RDLIGN are the rate constants for carbohydrates (an average for sugars and proteins), cellulose and hemi-cellulose, and lignin, respectively. In this formulation, the three components are assumed to comprise 20%, 70% and 10% of the original material, respectively.

$$\mathrm{CNRF}_i = e^{-.693 * (\mathrm{ACNR}_i - 25)/25},\ \mathrm{CNRF}_i \leqq 1 \tag{41}$$

(Parnas, 1975)

$$\mathrm{ACNR}_i = \mathrm{FRC} * \mathrm{FOM}_i/(\mathrm{FON}_i + \mathrm{ASLT}_i) \tag{42}$$

where

FRC = fraction carbon in fresh organic material

TF = temperature factor (Beek and Frissel, 1973) dependent on mean soil profile temperature, an approximation that may not be appropriate for the top soil layer

MF_i = moisture effect on decomposition rate, dependent on fraction of available water. Adapted from Hagin and Amberger (1974) and Been and Frissel (1973).

CNRF_i = effect of overall ratio of carbon and nitrogen on decomposition rate, - reduces the rate when the C:N ratio is above 25

ACNR_i = the C:N ratio based on nitrogen both in the organic and inorganic fraction.

The stable organic material, which has a constant C:N ratio of 10, is decomposed at a much slower rate, dependent on moisture and temperature conditions. A rate constant for semi-arid conditions is adopted from Harpaz (1975).

There is also an accretion of humus due to the residual stable compounds left by the decomposition process. In PAPRAN, this occurs after the C:N ratio is below 25. Only then is mineral nitrogen released and of that, 20% is incorporated into the stable fraction. Van Veen (1977) found values for microbial biomass 10-50 g m^{-2} in the top 15 cm soil layer. This is about 1-5 g m^{-2} nitrogen. Fresh organic nitrogen added annually is in the order of

1-10 g m^{-2}. These are similar values as for the microbial biomass. Of the latter, 25-60% is incorporated in the biologically stable humic compounds (Mayaudon and Simonart, 1963), with a relatively constant C:N ratio. This seems high for soils where the humic fraction is more or less stable. The C:N ratio of humus is taken as 10.
The net change in the amount of humus, $IHUM_i$, is thus,

$$IHUM_i = 0.2 * RNRL_i/NCH - RHMIN_i * 10 \tag{43}$$

where

$RNRL_i$, $RHMIN_i$ = see Eqns. (46) and (48)
NCH = nitrogen content of humus (0.04).

c. Soil nitrogen processes:

Soil nitrogen is divided into three fractions: nitrogen in the fresh organic material, in the stable organic material, and the mineral nitrogen. The change in fresh organic nitrogen is calculated as follows:

$$DFON_i = RNAC_i - RNRL_i \tag{44}$$

where

$RNAC_i$ = immobilization rate of mineral nitrogen by growing micro-organisms that decompose the fresh organic material (kg ha^{-1} day^{-1}, N)
$RNRL_i$ = rate of mineralization of nitrogen. Transfers N from FON to mineral pool (nitrate-N) and to the stable organic fraction (kg ha^{-1} day^{-1}, N).

$$RNAC_i = AMIN1\ (DECR_i * (NREQ - IFON_i/IFOM_i),\ ASLT_i/DELT) \tag{45}$$

NREQ = 0.02 (= fraction C in FOM (=0.4) * biosynthesis efficiency (=0.4/C:N ratio of microbial biomass (= 8)).

The biosynthesis efficiency of cellulose (Sörensen, 1975) is between 33-46%; it is not certain that it is a constant, but it is so used here. Equation (45) states that decomposition of 1 gram of fresh organic material (that includes the microbial biomass) will have to recruit (0.02 - IFON/IFOM) g of nitrogen. In the case of cellulose-rich and nitrogen-poor material, the nitrogen concentration, FNOM, is around 0.005, so that net release of nitrogen will begin when FNOM = 0.02 - 0.005 = 0.015, which is equivalent to a C:N ratio of 0.4/0.015 = 27. This is within the generally reported switching range for soil organic matter. The higher the initial nitrogen concentration, IFON/IFOM, the higher the threshold C:N ratio for net release of nitrogen, which is accordance with data quoted by Van Veen (1977).

Gross nitrogen release, $RNRL_i$, is then:

$$RNRL_i = DECR_i * FNOM_i \tag{46}$$

Gross release is thus dependent on the nitrogen concentration of FOM, but net release of N is due to decomposition of the microbial component of the fresh organic material. This assumes that the microbial population is in a steady state throughout the main decomposition period and is not per se limiting the rate of decomposition.

Change in the amount of nitrogen in the humic fraction is:

$$DNHUM_i = 0.2 * RNRL_i - RHMIN_i \tag{47}$$

$$RHMIN_i = NHUM_i * DMINR * TF * MF_i \tag{48}$$

DMINR = mineralization rate constant of stable organic material.

Change in amount of mineral nitrogen is:

$$DASLT_i = SLTF_i - SLTF_{i+1} - RNUM_i - RNUDB_i + 0.8 * RNRL_i - RNAC_i + RHMIN_i - RVOL_i \tag{49}$$

$$SLTF_i = RWF_i * CONC_{i-1} \tag{50}$$

$$SLTF_1 = NBR + FERTN \tag{51}$$

$$RWF_i = AMAX1\ (0., RWF_{i-1} - (FLDCP * THCKN_{i-1} - WATER_{i-1})/DELT \tag{52}$$

$$RWF_1 = INFR \tag{53}$$

$$RDRAIN = RWF_{N+1} \tag{54}$$

$$SLTFD = SLTF_{N+1} \tag{55}$$

$$CONC_i = (ASLT_i + (RWF_i * CONC_{i-1} - RNAC_i) * DELT)/(WATER_i + RWF_i * DELT) \tag{56}$$

where

$SLTF_i$ = rate of flow of nitrogen into soil layer i (kg ha^{-1} day^{-1}, N). Flow into the top layer is the sum of nitrogen borne in the rainfall, NBR, and fertilizer nitrogen applied, FERTN.

RWF_i = rate of water flow into compartment i (mm day^{-1}, H_2O); equivalent to excess above field capacity in previous compartment. Flow into first compartment is the infiltration rate of rain water, INFR.

$CONC_i$ = concentration of nitrogen in compartment i, that will flow out into the next compartment, includes the inflow of nitrogen and water from the previous compartment
RDRAIN = rate of deep drainage, equal to rate of water flow through last boundary
SLTFD = rate of leaching of nitrogen beyond rooting zone.

Volatilization rate of nitrogen, $RVOL_i$, from ammonia in the top soil layer is calculated by a mimicking procedure:

$$RVOL_i = (AMM1/TCV) * AMRF \tag{57}$$

$$AMM1 = ASLT_1 * (1 - RANO3) \tag{58}$$

$$AMRF = AMM1/LNH4', \ 0 \leq AMRF \leq 1 \tag{59}$$

$$RANO3 = INTGRL\ (0., (1-RANO3)/TCN) \tag{60}$$

where

AMM1 = amount of ammonia nitrogen in top layer when urea or ammonia fertilizer is applied (kg ha^{-1}, N)
AMRF = ammonia availability reduction factor, reduces volatilization as amount of ammonia in the top layer drops below a threshold level, LNH4
RANO3 = ratio of nitrate to ammonia nitrogen in the mineral fraction
TVC = time constant for volatilization of ammonia in top soil layer
TCN = time constant for nitrification.

Clearly, this representation of volatilization has very limited application and is entered here only because of a specific problem that was encountered.

D. *Soil water balance*

The conceptual background for the treatment of the soil-water balance in PAPRAN, is given in detail by Van Keulen (1975). The rate of change in the water status of each soil layer is:

$$DWAT_i = RWF_i - RWF_{i+1} - TRR_i - ER_i$$

where

TRR_i = contribution of layer i to crop transpiration (mm day^{-1}, H_2O)
ER_i = contribution of layer i to evaporation from the soil surface (mm day^{-1}, H_2O).

8. PARAMETERS AND FUNCTION TABLES

A. *Soil parameters and initial values*

WLTPT	wilting point, cm^3 cm^{-3} (= 0.075 for sandy loam, Gilat loess)
FLDCP	field capacity, cm^3 cm^{-3} (= 0.23 for sandy loam, Gilat loess)
B	soil surface water storage capacity, mm (= 5)
THCKN$_i$	thickness of soil layers, mm (i_{1-10} = 20, 30, 50, 100, 100, 5 * 300)
DRF$_i$	initial dryness factor - soil moisture in multiples of WLTPT
IAS$_i$	initial amount of mineral nitrogen (as nitrate), kg ha^{-1}, N
FOMI	initial amount of plant residues, 'fresh organic material', kg ha^{-1}, d.m.
FONI	initial amount of nitrogen in fresh organic material, kg ha^{-1}, N
HUMI	initial amount of stable organic material, 'humus', kg ha^{-1}, d.m.
NHUMI	initial amount of nitrogen in stable organic fraction, kg ha^{-1}, N
DFFOM$_i$	initial distribution of organic material and organic nitrogen among the layers of the soil profile. It is assumed that no active organic material occurs below 600 mm depth.
FRNF	initial fraction of nitrogen in the fresh organic material
FRC	fraction of carbon in the plant residues (= 0.4)
NGIFT	rate of nitrogen fertilizer application, kg ha^{-1}, N
NDAY	day of nitrogen fertilizer application
NCR	nitrogen concentration in the rain, kg mm^{-1} ha^{-1}, N (= 0.02)
RDCAR	decomposition rate constant for sugar and proteins, day^{-1} (= 0.8)
RDCELL	decomposition rate constant for cellulose and hemi-cellulose, day^{-1} (= 0.05)
RDLIGN	decomposition rate constant for lignin, day^{-1} (= 0.0095)
DMINR	decomposition rate constant for stable organic material, day^{-1} (= 8.3 * 10^{-5})

B. *Vegetation parameters and initial values*

IBIOM	initial biomass after establishment of vegetation at the beginning of growing season, kg ha^{-1}, d.m.
IWRT, WLVSI, WNLVSI	initial weight of roots, leaves and non-leaf material; functions of IBIOM, kg ha^{-1}, d.m.
IRTD	initial root depth after establishment of vegetation, mm (= 101)
IANS	initial amount of nitrogen in the seed; function of the optimum nitrogen concentration in the seed and the growth rate of the seed, GRSDS, at the onset of seed fill
MXRTD	maximum rooting depth, mm (1800 for natural vegetation)
DGGRT	daily maximum root growth rate, mm day^{-1} (= 12.0)
DVSSF	development stage for onset of seed fill (= .65)
AMAXB	maximum rate of CO$_2$ assimilation, kg ha^{-1} (leaf) h^{-1}, CO$_2$ (= 40)
EFFEB	maximum efficiency of radiation utilization (kg ha^{-1})/(J m^{-2} s^{-1}), CO$_2$ (= 0.5)
MRESF	maintenance respiration factor, kg (CH$_2$O) kg^{-1} (d.m.) (= 0.02)
REFT	reference temperature at which MRESF holds for maintenance respiration, °C (= 25)

CONFS	conversion efficiency of carbohydrate to plant dry matter (= 0.75)
FWDB	fraction of water in dead plant biomass, kg (H_2O) kg^{-1} (d.m.) (= 0.90)
LFARRS	standard leaf area ratio, m^2 kg^{-1} (= 20)
LN	threshold nitrogen concentration below which growth stops, kg (N) kg^{-1} (d.m.) (= 0.005)
ONCH	optimum nitrogen concentration in seeds at onset of seed fill, kg (N) kg^{-1} (d.m.) (= 0.045)
ONCL	optimum nitrogen concentration in seeds at maturity, kg (N) kg^{-1} (d.m.) (= 0.025)
MNU	maximum nitrogen uptake rate by roots when vegetation fully developed ('closed canopy') kg ha^{-1} day^{-1} (= 9)

C. *Constants*: physical and biological

REFCF	reflection coefficient of water (= 0.05)
LHVAP	latent heat of vaporization of water, cal mm^{-1} (= 59)
GAMMA	psychrometric constant, mm $^oC^{-1}$, Hg (= 0.49)
RHOCP	volumetric heat capacity of air, cal cm^{-3} $^oC^{-1}$ (= $2.86 * 10^{-4}$)
RS	stomatal resistance, day cm^{-1} (= $18.5 * 10^{-6}$ = 160 s m^{-1})
RC	cuticular resistance, day cm^{-1} (= $37 * 10^{-5}$ = 3200 s m^{-1})
PSCH	psychrometric constant, mbar $^oC^{-1}$ (= 0.67)
LNH_4	threshold nitrogen content in soil above which volatilization is not restricted by available ammonia kg ha^{-1}, N (= 2.2)

D. *Time constants*

TAU2	demand for nitrogen in the plant (= 2)
TCV	volatilization of ammonia applied as fertilizer to the surface soil layer (= 10)
TCN	nitrification of fertilizer ammonia (= 10)
TCDRL, TCDRNL	dying rate of leaves and non-leaf material due to water shortage

E. *Weather*: entered as forcing functions dependent on time

DTR	daily total global radiation, cal cm^{-2} day^{-1}
MNT	minimum air temperature, ^oC
MXT	maximum air temperature, ^oC
WS	average daily windrun, kg day^{-1}
DPT8	dew point temperature at 08.00 hrs, ^oC
DPT2	dew point temperature at 14.00 hrs, ^oC
RAIN	daily rainfall, mm day^{-1}
RADTB	total daily visible radiation on clear days as a function of latitude and time of year, cal cm^{-2} day^{-1}

These data are used to obtain auxiliary variables applied in the model:

TMPA = average air temperature, ^oC
EVAP = potential evaporation, mm day^{-1}, H_2O

F. *Environmental effects on soil and plant processes*

These are entered in tabulated form:

a. Functions dependent on soil moisture

WREDT	f(AWATER$_i$), relation between fraction of available soil water and root water uptake
EDPTFT	f(AWATER$_i$), effect of fraction of available soil water on root effectiveness for water uptake
REDFDT	f(WCPR), (= dimensionless water content = (WATER$_1$/THCKN$_1$ - WCLIM)/(FLDCP - WCLIM) where WCLIM = water content of air-dry soil) reduction of bare soil evaporation due to dryness of the top soil layer
MFT	f(WATER$_i$), effect of soil water content on decomposition rate of fresh organic material

b. Functions dependent on soil temperature

REDTTB	f(TS), soil temperature effect on root extension rate
TECT	f(TS), soil temperature effect on root conductivity
TFT	f(TS), soil temperature effect on decomposition rate of fresh and stable organic material

c. Functions dependent on nitrogen concentration

ROSPT	f(CONC$_i$), effect of ionic concentration in soil water on root water uptake
FANST	f(N in vegetation), effect of nitrogen deficiency on partitioning of assimilate between leaves and non-leaf material

d. Functions dependent on development stage of the vegetation

RFDVST	f(DVS), effect on transpiration as plant matures
DISTFT	f(DVS), effect on distribution of assimilate between leaf and non-leaf material
CSRRT	f(DVS), effect on distribution of assimilate between shoot and root
FDMT	f(DVS), effect on dry matter content of the live vegetative biomass (phytomass)
RDRDT	f(DVS), effect of senescence on the dying rate of live phytomass
MFRTT	f(DVS), maximum fraction of nitrogen in the root

e. Functions dependent on air temperature

DVRT	f(TMPA), effect of average air temperature on development rate of vegetation

f. Functions dependent on transpiration deficit

RDRAT	f(CTRDEF), effect of cumulative transpiration deficit on AMAX and EFFE
FAMSTT	f(RTRDEF), effect of relative transpiration deficit on partitioning of assimilates between roots and shoots

g. Functions dependent on the vegetation canopy

FLTRT f(SLCVR) (= total area of live and dead leaf per hectare), effect of canopy closure on the amount of radiant energy that reaches the soil surface, calculated as 1 - C, where $C = e^{-0.5 * LAI}$ (Goudriaan, 1977)

h. Functions dependent on radiation intensity and leaf area index

ALPHA f(HRAD, LAI), effect of radiation and leaf area on the potential transpiration demand of the canopy. This is entered as a two way table, derived from the plant physiological model BACROS (De Wit et al., 1978)

9. OUTPUT: VERIFIABLE VARIABLES

a. TADRW: Total above-ground dry matter as a function of time. In some situations, validation data were available for final yields only, a serious limitation in analyzing deviations of model results from observed data.

b. WLVS, WMLVS and WSDS: the weight of leaves, non-leaf material and reproductive structures. These variables are generally available for crop plants but not for natural pasture species (De Ridder, Seligman and Van Keulen, 1980).

c. TNLVS, TNNLVS, ANS: the total amounts of nitrogen in various plant organs. The sum of these will give total nitrogen uptake by the above ground parts of the canopy.

d. $W_1 \ldots W_{10}$: the moisture content of the various layers of the soil. Since soil water dynamics are not treated in great detail in PAPRAN, it may be more realistic to use only WTOT, total moisture in the potential rooting zone, for validation.

e. $ASLT_1 - ASLT_{10}$: the amounts of inorganic nitrogen in the various soil compartments.

f. HUM, NHUM, FOM, FNOM: the amounts of organic matter in the soil and their nitrogen contents (or C:N ratio) are available for validation also. A serious difficulty is that the experimental techniques available for determination of these state variables, do not in general permit a high accuracy. Since the amounts involved can be high (HUM = 28000 kg ha^{-1}, NHUM = 2800 kg ha^{-1} in the Northern Negev) almost any number simulated will fall within the accuracy limits. The model may, however, give trends for the behaviour of soil organic matter, which may be evaluated over a number of years.

10/11. OBSERVATIONS AND COMPARISON RESULTS

The performance of the model was studied by analysing its behaviour under conditions prevailing in the northern Negev desert of Israel. In this semi-arid region (average rainfall 250 mm $year^{-1}$) research has been carried out in the framework of a joint Dutch-Israeli project (Van Keulen and De Wit, 1975). From this and earlier research (Tadmor et al., 1974) results are available of dry matter yields in situations with and without application of nitrogenous fertilizer. These experiments were carried out on the natural vegetation of the area which is a mixture of plant species, typical of an abandoned crop land vegetation (Van Keulen, 1975).

The initial conditions assumed in the model were identical for all seasons: at the onset of the growing season a total amount of 3000 kg fresh organic material was assumed to be present in the upper 60 cm of the profile. The average nitrogen content of the material was set at 0.01 kg N kg^{-1} (dry matter). When fertilizer was added in the model, this was also assumed to be present at the onset of the simulation, in ammoniacal form, evenly distributed in the upper 10 cm of the soil. The initial moisture conditions in the profile were either those measured (1971/1972 - 1973/1974) or were estimated at an average value (1966/1967 and 1967/1968).

The results of the model are presented in Figs 2-6 in the form of results of fertilizer experiments. The available experimental data are given for comparison. This gross output does not show a consistent picture:

- For 1966/1967, where only application-yield data were available, the yield without additional fertilizer application is reasonably well estimated. The simulated response curve deviates however from the measured one: at low application rates the effect of additional fertilizer is overestimated, whereas the maximum experimental yield exceeds the predicted one. The latter value is identical to that obtained from the model ARID CROP (Van Keulen, 1975) which assumes non-limiting nutritional conditions throughout.

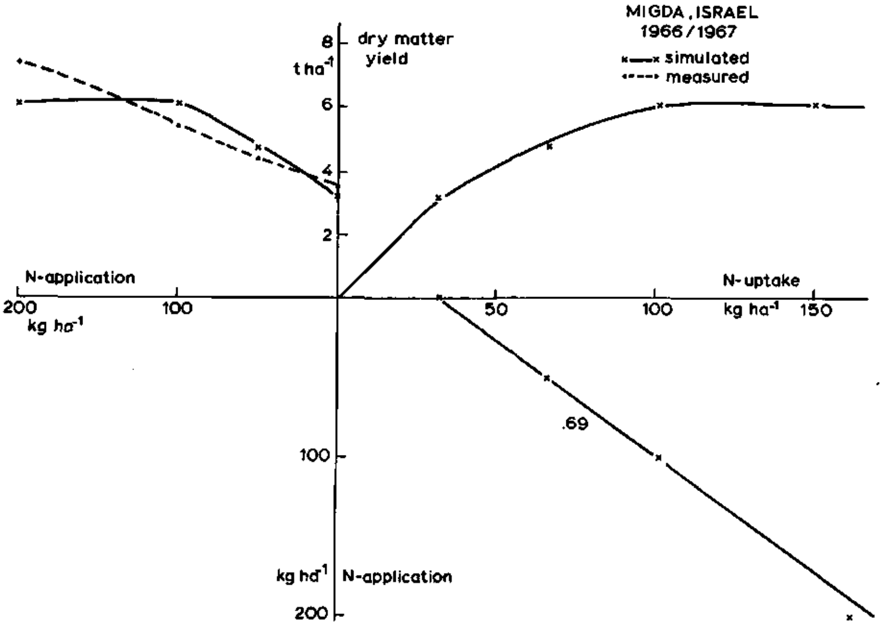


Fig. 2. Comparison between measured and simulated results of a fertilizer experiment in the Northern Negev in 1966/1967.

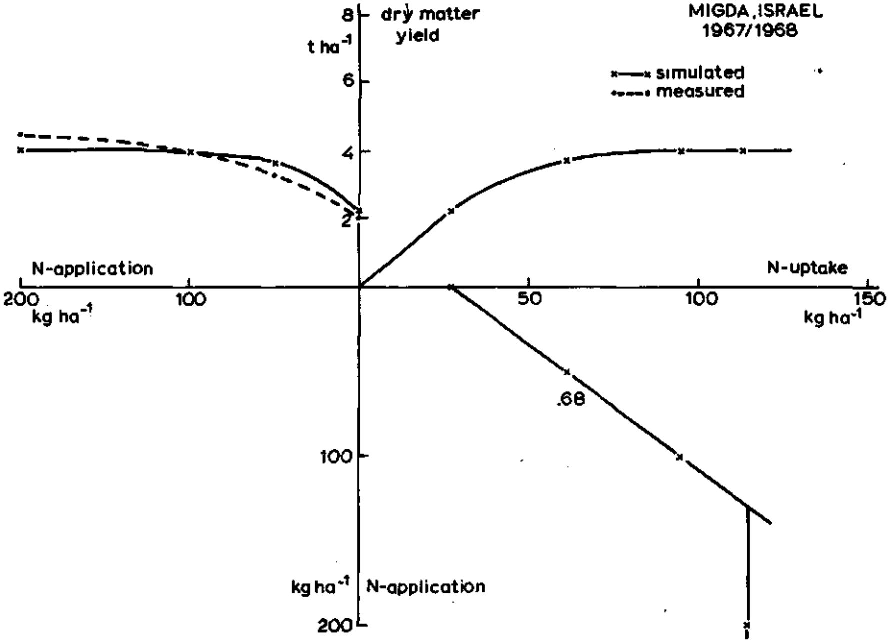


Fig. 3. Comparison between measured and simulated results of a fertilizer experiment in the Northern Negev in 1967/1968.

- For 1967/1968, a lower rainfall year, the simulated yield-application curve is reasonably close to the measured one over the entire range. Because of the drier conditions, decomposition of the added organic material is less complete than in the previous season and consequently about 5 kg N ha^{-1} less is available at zero-fertilizer application, resulting in about a one ton lower dry matter production.
- For 1971/1972 the various experimental treatments resulted in the uptake of varying amounts of nitrogen. A 'true' zero-treatment could not be analysed in that season, since the experimental fields were all disked, thus incorporating into the soil substantial amounts of accumulated sheep droppings from preceding seasons. The amounts and composition of these droppings cannot be estimated, hence it is impossible to account for their effect on the nitrogen balance. The simulated uptake-yield curve is situated within the accuracy-limits of the measured data points. At the highest application rate the model predicts a levelling off of the application-uptake curve, since the crop is 'nitrogen-saturated' throughout the growing season. The predicted amount is again in reasonable agreement with the experimentally determined uptake.
- For 1972/1973 the experimentally determined points of the yield-uptake curve deviate considerably from the simulated curve. There is no obvious explanation for this phenomenon. The measured maximum uptake of nitrogen is about 25% higher than that predicted by the

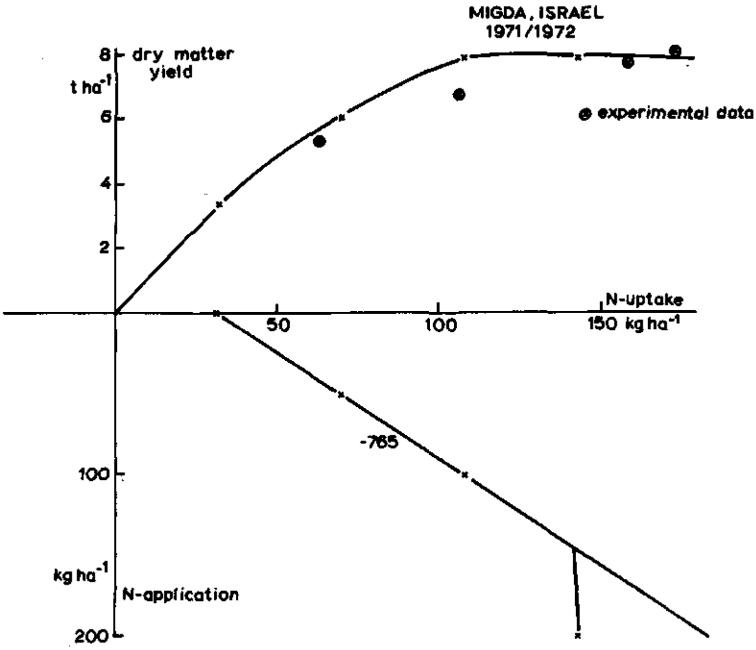


Fig. 4. Comparison between measured and simulated values of dry matter production and nitrogen uptake of natural vegetation in the Northern Negev in 1971/1972.

model, which was again dictated by the ability of the vegetation to absorb the element.

- For the 1973/1974 growing season only the fully fertilized treatment was analysed for nitrogen at the end of the growing season. The point found there, shows a higher uptake than the maximum predicted by the model, as in the previous season. In the lower region no data are available.

More interesting than the gross output of the model at this stage, is the behaviour of some of its elements.

The fresh organic matter assumed to be present at the start of the growing season decomposes almost completely, 5-15% being left at the end of the growing period. It should be noted, that the relative decomposition rates of the various components, applied in the model are an order of magnitude higher than those cited by Beek & Frissel (1973). Application of their values leads to unrealistically low decomposition rates.

Concurrently with the decomposition of the organic material there is a slow but gradual release of mineral nitrogen when the original (protein) nitrogen concentration in the organic material is 0.01 kg (N) kg^{-1} (d.m.). When material with a lower initial protein nitrogen content (FNRF) is assumed, there is net immobilization at first, later followed by net mineralization (Fig. 7).

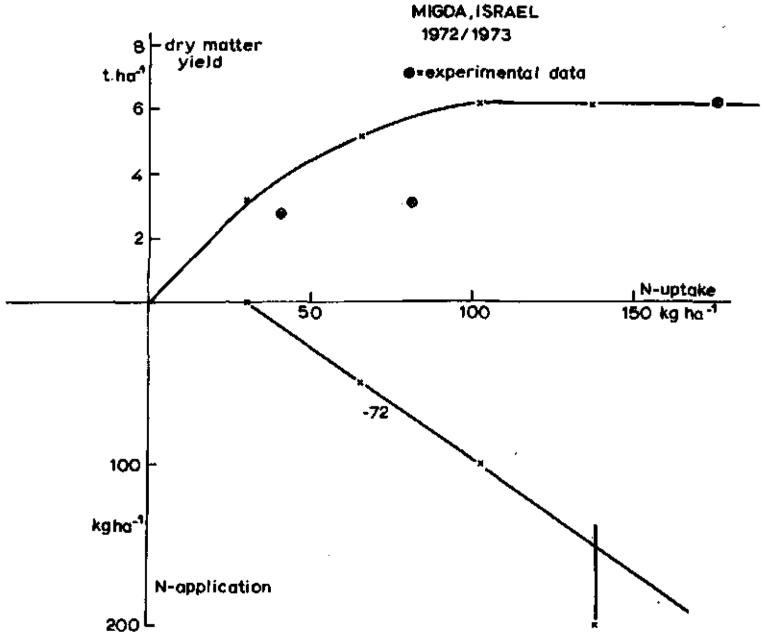


Fig. 5. Comparison between measured and simulated values of dry matter production and nitrogen uptake of natural vegetation in the Northern Negev in 1972/1973.

An important question in this connection is, whether it is possible to describe quantitatively the nitrogen transformations in the soil, and their consequences for the availability of the element for plant uptake, without explicitly describing the microbial population. The problems related to the description of that part of the nitrogen cycle have been mentioned before and have been discussed in detail by Van Veen (1977). Additionally there is the inaccuracy of the experimental techniques for the determination of the various components of the total nitrogen store in the soil, and the inherent heterogeneity of the system under field conditions. It is expected that current field experiments employing N^{15} will yield results, which will at least elucidate some of the problems.

The effects of nitrogen deficiency on various plant processes had to be estimated in many cases on the basis of incomplete and qualitative rather than quantitative information. At this stage no attempt has been made to test the sensitivity of the model to the various estimated relations. Some remarks seem warranted however:

- the influences of nitrogen deficiency on dry matter accumulation is introduced as a reduction factor on the growth rate. The underlying physiological reason, which could either be a direct effect of low N-concentration on assimilation, or an indirect effect through accumulation of primary photosynthates in the leaf tissue, or a lower efficiency of growth due to breakdown and rebuilding of nitrogenous compounds, is not completely understood, so that a more fundamental explanatory representation is not yet feasible.

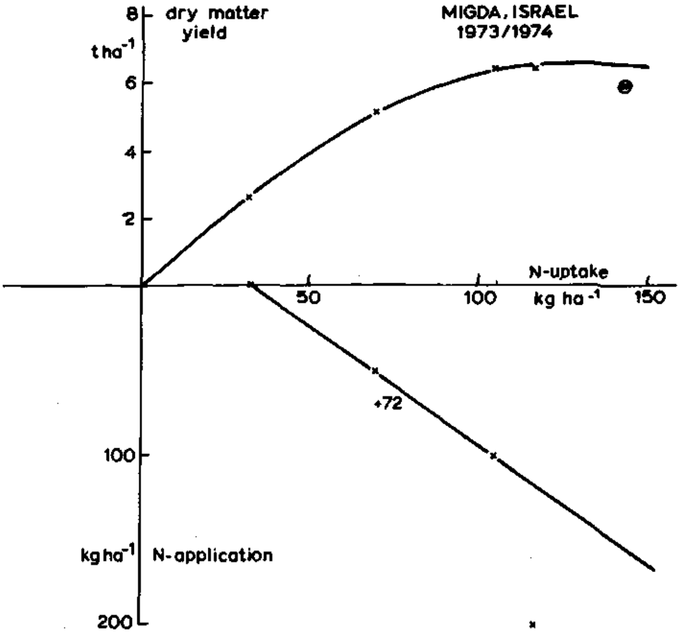


Fig. 6. Comparison between measured and simulated values of dry matter production and nitrogen uptake of natural vegetation in the Northern Negev in 1973/1974.

The use of another relation between the relative death rate and the nitrogen content of the vegetation (i.e. curvilinear in the opposite direction), resulted for the 1966/1967 growing season in decreased productivity at higher N-applications. This was caused by the interaction between nitrogen and water: N-shortage early in the season resulted in dying of part of the vegetation, leading to lower water extraction and increased growth at the end of the growing period. The phenomenon as such has been discussed widely in connection with dry-land agriculture, but for the 1966-1967 situation it is not confirmed by the experimental results. These results however underline the necessity for a more systematic investigation of the relative importance of the various processes that play a role under these conditions.

In conclusion it may be stated that PAPRAN does provide a useful framework for such an investigation. It is realized, that at many points the model is descriptive rather than explanatory and needs a more thorough validation before it can be widely applied.

12. LIMITS AND LIMITATIONS

PAPRAN is meant to deal with problems relating to seasonal and interseasonal dynamics of plant production processes. A time constant of days is 2 to 3 orders of magnitude smaller than the seasonal relaxation time. That is just about the limit for feasible simulation modelling of biological systems (De Wit, 1970). Accordingly the time step for PAPRAN

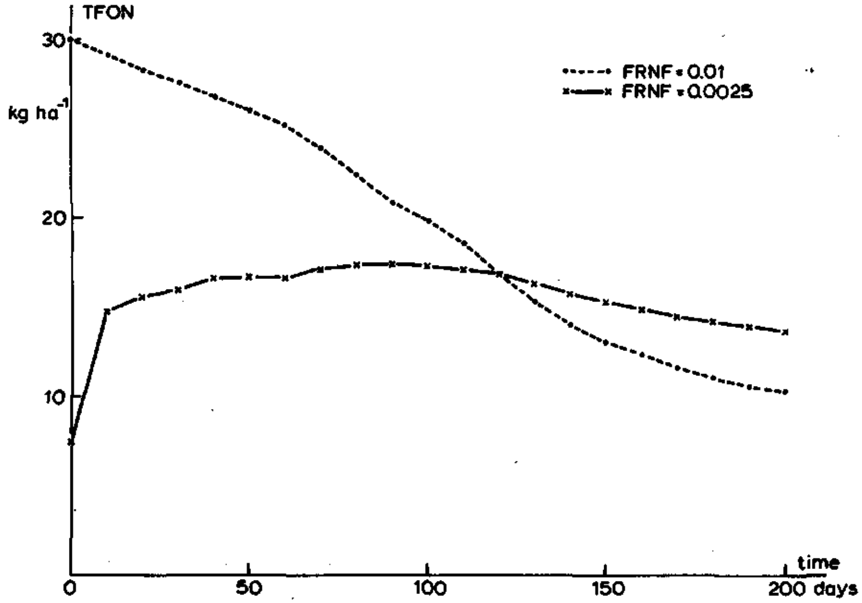


Fig. 7. The influence of the initial nitrogen concentration of the added organic material (FRNF) on the amount of nitrogen retained in the fresh organic fraction (TFON).

has been set to one day. It is a constant time step and cannot be varied without extensive rewriting of parts of the program. As a result processes having a time resolution smaller than one day cannot easily be incorporated into this model. If a given problem is critically dependent on the exact description of such processes, it would be necessary to resort to another model, with finer resolution and more limited scope. The results of this model could be later incorporated into the lower resolution model, according to the hierarchical approach.

Finally, some processes have been ignored in PAPRAN:

- denitrification is disregarded because in semi-arid regions anaerobic conditions are unlikely. The possibility that localised anaerobic pockets can develop as a result of oxygen depletion due to intensive biological activity or localised waterlogging is recognized but as the extent of these phenomena is not clear, they have not been treated as yet. In addition, the problem of simulating localised anaerobiosis in soils is particularly complex (Leffelaar, 1979).

13. COMPUTER

As the model is written in CSMP III, it can only be run on systems that have that language available. Those are generally IBM-machines except for some cases where the language has been specially adapted for a different computer system.

14. PROGRAM LANGUAGE

The program is written in CSMP III, the Continuous System Modelling Program, developed by IBM (1971).

15. RUNNING TIME

To simulate one growing season, about 40 secs CPU-time is required. This includes the time needed for translation and compilation of the original CSMP Program. Reruns in the same case take usually less than 10 secs CPU-time. In most installations the CSMP-program can be stored in compiled form for running from execution phase. In that case CPU-time for the first run is nearly the same as reruns within one case, i.e. about 10 secs.

Costs of a run depend on local billing arrangements, but in any case they depend very much on the amount of output required.

16. USERS

The model is still being developed and has been used only within the joint Dutch-Israeli project: Actual and potential production from semi-arid grassland-phase II. It has also been run on an explanatory basis within a companion project: Production Primaire au Sahel (PPS), that is concerned with growth of Sahelian natural pasture in Mali.

17. DEVELOPERS AND PRINCIPAL CONTACTS

Dr. H. van Keulen
CABO
P.O. Box 14, Wageningen, The Netherlands

Dr. N.G. Seligman
A.R.O. Volcani Center
P.O. Box 6, Bet Dagan, Israel

REFERENCES

Bartholomew, W.V., and F.E. Clark, 1965. Soil nitrogen, Agronomy 10, American Society of Agronomy, Madison, Wisc.

Beek, J., and M.J. Frissel, 1973. Simulation of nitrogen behaviour in soils. Simulation Monographs, Pudoc, Wageningen.

Dobben, W.H. van, 1961. Nitrogen uptake of spring wheat and poppies in relation to growth and development. Jaarboek I.B.S. 1961: 54-60 (Dutch with English summary).

Dijkshoorn, W., D.J. Lathwell, and C.T. de Wit, 1968. Temporal changes in carboxylate content of ryegrass with stepwise change in nutrition. Plant and Soil 29: 369-390.

Feigin, A., and D.H. Yaalon, 1974. Non-exchangeable ammonium in soils of Israel and its relation to clay and parent material. Journal of Soil Science 25: 384-397.

Goudriaan, J., 1977. Crop micrometeorology: a simulation study. Simulation Monographs, Pudoc, Wageningen.

Goudriaan, J., and H.H. van Laar, 1978. Relations between leaf resistance, CO_2 concentration and CO_2 assimilation in maize, beans, lalang grass and sunflower. Photosynthetica 12: 241-249.

Goudriaan, J., and H. van Keulen, 1979. Direct and indirect effects of nitrogen shortage on assimilation and transpiration in maize and sunflower. Netherlands Journal of agricultural Science 27: 227-234.

Hagin, J., and A. Amberger, 1974. Contribution of fertilizer and manures to the N- and P-load of waters. A computer simulation. Deutsche Forschungsgemeinschaft, Bonn, Technion Research and Development Foundation Ltd. Haifa.

Harpaz, Y., 1975. Simulation of the nitrogen balance in semi-arid regions. Ph.D. Thesis Hebrew University, Jerusalem.

IBM, 1971. Continuous System Modelling Program III. IBM Technical Report GH 10-7000-1.

Jansson, S.L., 1958. Tracer studies on nitrogen transformations in soil with special attention to mineralization-immobilization relationships. Kungl. Lantbr. Ann. 24: 101-136.

Keulen, H. van, 1975. Simulation of water use and herbage growth in arid regions. Simulation Monographs, Pudoc, Wageningen.

Keulen, H. van, and C.T. de Wit, 1975. Actual and potential herbage production in arid regions - an annotated bibliography. Report Department of Theoretical Production Ecology, Agricultural University, Wageningen.

Keulen, H. van, N.G. Seligman, and J. Goudriaan, 1975. Availability of anions in the growth medium to roots of an actively growing plant. Netherlands Journal of agricultural Science 23: 131-138.

Keulen, H. van, N.G. Seligman, and R.W. Benjamin, 1980. Simulation of water use and herbage growth in arid regions - re-evaluation and further development of the model ARID CROP, Agricultural Systems (in press).

Kononova, M.M. 1961. Soil organic matter. 2nd English edition. Pergamon Press, London.

Krul, J., 1980. Personal communication.

Leffelaar, P.A., 1979. Simulation of partial anaerobiosis in a model soil in respect to denitrification. Soil Science 128: 110-120.

Mayaudon, J., and P. Simonart, 1963. Humification des micro-organismes marqués par ^{14}C dans le sol. Annales Institute Pasteur 118: 191-198.

Parnas, H., 1975. Model for decomposition of organic material by micro-organisms. Soil Biology and Biochemistry 7: 161-169.

Penman, H.L., 1948. Natural evaporation from open water, bare soil and grass. Proceedings Royal Society London, A 193: 120-146.

Ridder, N. de, N.G. Seligman, and H. van Keulen, 1980. The reproductive effort of annual pasture species in grazed and ungrazed swards (Oecologia (Berlin), submitted).

Russel, P.E., 1958. Soil conditions and plant growth. 8th edition. Longmans, London.

Seligman, N.G., H. van Keulen, and J. Goudriaan, 1975. An elementary model of nitrogen uptake and redistribution by annual plant species. Oecologia (Berlin) 21: 243-261.

Sörensen, L.H., 1975. The influence of clay on the rate of decay of ammonia acid metabolites synthesized in soils during decomposition of cellulose. Soil Biology and Biochemistry 7: 171-177.

Tadmor, N.H., E. Eyal, and R.W. Benjamin, 1974. Plant and sheep production on semi-arid grassland in Israel. Journal of Range Management 27: 427-432.

Tandon, H.L.S., 1974. Dynamics of fertilizer nitrogen in Indian soils. I. Usage, transformation and crop removal of N. Fertilizer News 19: 3-11.

Veen, J.A. van, 1977. The behaviour of nitrogen in soil. A computer simulation model. Ph.D. Thesis. University of Amsterdam.

Wit, C.T. de, 1958. Transpiration and crop yields. Verslagen landbouwkundig Onderzoek (Agricultural Research Reports) 64.6; Pudoc, Wageningen.

Wit, C.T. de, 1970. Dynamic concepts in biology. Proc. IBP/PP Technical Meeting, Trebon, Pudoc, Wageningen.

Wit, C.T. de, et al., 1978. Simulation of assimilation, respiration and transpiration of crops. Simulation Monographs, Pudoc, Wageningen.

4.11 Models of long term soil organic nitrogen change

J.S. Russell

INTRODUCTION

Long term soil organic nitrogen dynamics are of considerable interest in agro-ecosystems. Aspects such as equilibrium levels, rates of decline or increase with time, crop yield trends and feedback effects of increased crop yields on soil organic matter due to fertilizer addition are interrelated. Mathematical modelling has an important role to play in understanding these interactions and in predicting consequences of land use practices.

There are a number of difficulties in modelling long term soil nitrogen changes as distinct from short term changes. Not the least of these is the fact that the time span of significant changes of 10 to 100 years makes experimental validation difficult. Also the diversity of climate, soils, crops, cropping sequences and cultivation and fertilization practices makes generalization difficult. Even when data is available for a long period from research stations it is generally site and soil specific. Nevertheless an analytical approach to such information is a starting point for defining factors affecting long term soil nitrogen changes and for the establishment of relationships and parameters which can be used in models. From there it is possible to move to relatively simple predictive models which can be useful in suggesting the outcome of various land use options.

ANALYTICAL APPROACHES USING FIELD DATA

There is an extensive literature on mathematical expression of soil organic matter with time (Jenny, 1941; Dawson, 1950; Nye and Greenland, 1960; Henin et al., 1959; Bartholomew and Kirkham, 1960; Russell, 1960, 1962, 1964, 1975; Jenkinson and Rayner, 1977).

The simplest model has been the differential equation:

$$dN/dt = -K_1N + K_2 \tag{1}$$

where N is soil organic nitrogen or carbon, K_1 is a decomposition coefficient and K_2 is an addition term. This equation has been useful in situations where a treatment has been used for a long period and where substantial soil changes have occurred e.g. grassland areas at Rothamsted (Richardson, 1938).

Extension of this equation can move logically in two directions. Firstly, a more sophisticated model needs to consider separate soil organic matter fractions and examine interactions and changes with time. Secondly to be useful, in land use terms, account needs to be taken of the interactions between crop-pasture sequences, soil organic matter and crop yield.

Mathematical models involving more detailed analysis of soil organic matter fractions were proposed by Woodruff (1949) and Henin et al., (1959). However, field fractional soil organic matter data was not available to develop these approaches further. Recently Jenkinson and Rayner (1977) separated soil organic matter into five fractions, decomposable plant material, resistant plant material, soil biomass, physically stabilized organic matter and chemically stabilized organic matter. They applied this approach to soils from Rothamsted classical experiments where soil analytical information is available over a period of more than 100 years and where different cropping and manuring treatments have been virtually continuous for longer than this. The model assumes that each of the fractions undergoes biological decomposition by a first-order process. From this study the authors were able to predict turnover of these fractions with time.

Soil organic nitrogen changes in crop-pasture sequences (Russell, 1975) were described by the general equation

$$dN/dt = -K_1(t)N + K_2 + K_3(t)Y(t) \qquad (2)$$

where $K_1(t)$ is the decomposition coefficient which may change with time as land is used for different crops and pastures. The term K_2 represents additions from non-crop sources, including farmyard manure. The term $K_3(t)Y(t)$ represents addition due to plant residues where $Y(t)$ refers to the crop yield at time t and $K_3(t)$ is related to a specific crop at time t.

The main advantage of such a model is that it can take into account the effects of various land use treatments and crop yields within a rotation on soil organic matter levels. Using plant and soil data it is possible to estimate the feedback effect of plant yield on soil organic matter level.

Various restrictions can be applied to equation (2) in practice to reduce the number of parameters to be estimated in fitting to experimental data. These can include assumptions that: (a) K_2 is zero, (b) the relationship between decomposition and addition coefficients is the same for all crops in the system

i.e. that $K_3/K_1 = a$

where a is a constant, (c) K_3 is the same for similar crops. Such assumptions can simplify the model and reduce the number of parameters to be estimated in an analysis.

Procedures for fitting the model to plant and soil data were described by Russell (1975) by making use of an iterative routine which numerically solves ordinary differential equations from a set of initial values and parameters over a desired period (Ross, 1973) combined with a routine which minimizes least squares for a set of actual data and calculated values from the mathematical model (Ross, 1971).

Given quantitative estimates of decomposition and addition parameters for different crops it is possible to simulate soil organic matter changes with various crop sequences and make predictions of long term effects.

MODEL OF EFFECT OF CROP-PASTURE ON SOIL ORGANIC NITROGEN

Crop-pasture sequences are used in semi-arid areas where low and variable rainfall limits the use of applied nitrogen (Russell, 1968). To increase crop yields fallowing[1] has been practiced (Sims, 1977) to allow a longer period of nitrogen mineralisation and to enable soil water from one season to be stored for plant growth in the following season. Whilst this practice achieves, it results in increased rates of soil organic nitrogen loss. A considerable number of field experiments have been carried out in Australia on the effects of crop-pasture sequences including fallow in different environments (Clarke and Russell, 1977) in relation to crop yield and soil nitrogen change.

One of the oldest continuing experiments in the permanent rotation trial established at the Waite Agricultural Research Institute (lat. 34°58'S long. 138°38'E) in 1925. This Institute has an annual rainfall of 629 mm, an annual evaporation of 1580 mm and an annual temperature of 16.4 °C. Rainfall is winter dominant with 77% falling in the period April to October.

The permanent rotation experiment has included a range of sequences but the main emphasis has been on the effects of fallow, wheat and pasture and combinations of these. Plant yield data has been meticulously recorded (e.g. various Waite Institute reports 1925-1975) but soil information is much less detailed (Greenland, 1962). Although this limits the extent to which soil-plant parameters can be accurately estimated, parameter estimation is aided by the very large changes in soil organic nitrogen that have occurred with time. Soil analyses in 1961 (Greenland, 1962) showed that some had lost up to 50% of organic nitrogen in the surface 23.5 cm. Soil analyses in 1973 (Russell and Oades, unpubl. data) showed that losses of organic nitrogen were continuing on some sequences.

To obtain parameters of soil organic nitrogen change size sequences of this experiment were studied and a model of the form

$$dN/dt = -K_1(t)N + K_3(t)Y(t) \qquad (3)$$

fitted to the soil data using annual plant dry matter yields. The sequences examined were fallow-wheat (FW)[2], fallow-wheat-pasture (FWP), fallow-wheat-pasture-pasture (FWPP), wheat-pasture-pasture (WPP), continuous wheat (WW) and continuous pasture (PP). Some of these sequences were continued over the period 1926-1973[3] but for others information was available only for the period 1949-1973. Four parameters were estimated including decomposition coefficients (in terms of % year^{-1}) for fallow (K_{1f}), wheat (K_{1w}) and pasture (K_{1p}) and a general addition coefficient (in terms of % N ha year^{-1} kg^{-1} (dry matter) related to dry

---

[1] Fallowing involves leaving land cultivated and devoid of vegetation for periods of up to a year, prior to cropping.

[2] Two plots of this sequence.

[3] FW, FWP and WW were continuous.

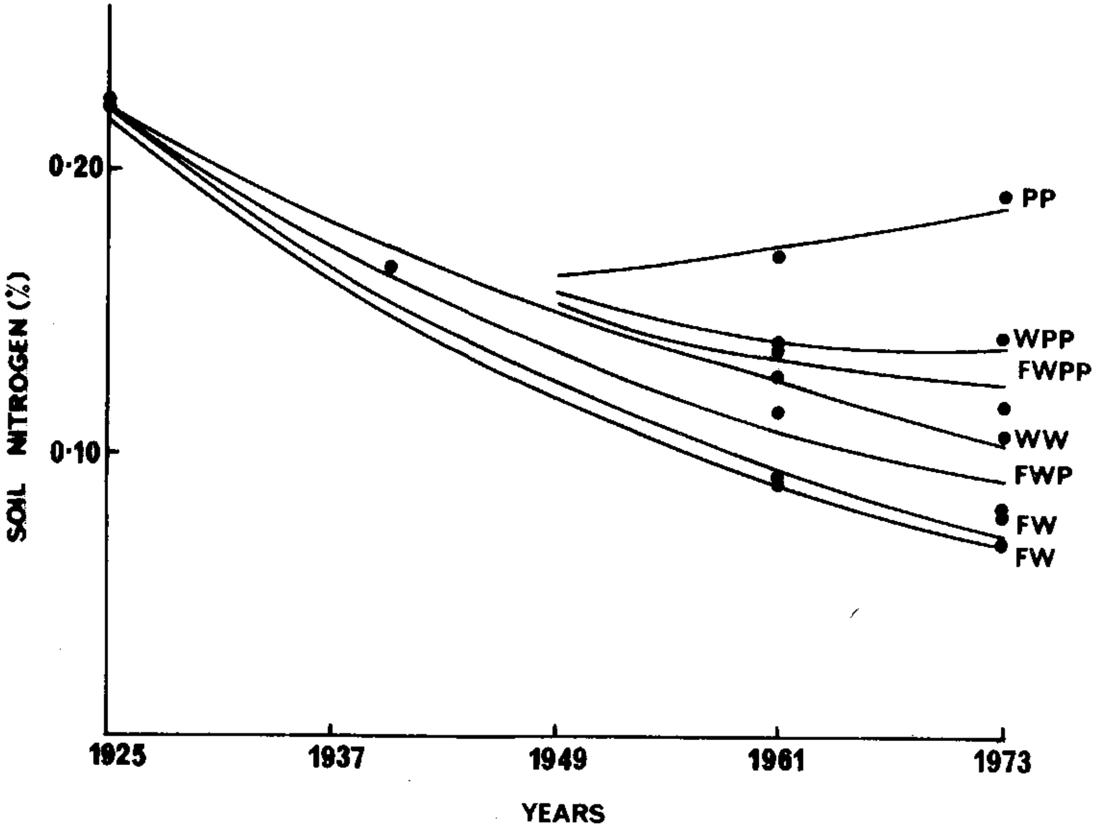


Fig. 1. Changes in the soil nitrogen content in fallow, wheat and pasture plots at the permanent rotation experiment at the Waite Institute, Adelaide, Australia and estimated changes using the fitted model.

matter production (K_{3dm}). The model was fitted to the 0-10 cm soil nitrogen data using 18 total soil nitrogen percentage values for 1925[1], 1940, 1961 and 1973. Estimated values of the coefficients were $K_{1f} = 0.0440$, $K_{1w} = 0.0253$, $K_{1p} = 0.0270$ and $K_{3dm} = 5.21 \times 10^{-7}$. The fit of the model to the data is shown in Figure 1. The model accounted for 99.0% of the variation about the mean.

With the coefficients it is possible to simulate the effects of various FWP sequences on soil organic nitrogen. Assumptions have to be made concerning crop yields and these are based on the long term (22-50 years) mean dry matter yields (Waite Institute Biennial Report, 1974-75). Values in kg ha^{-1} used in calculations were: wheat after fallow and after pasture 5100, second year wheat 3900, continuous wheat 2700, first year pasture 6100,

---

[1] Of the two 1925 FW values the high value similar to that of other treatments was used for both FW plots. The 0-10 cm portion of the 1925 0-23.5 cm values were estimated.

second year pasture 8800, third year pasture 10400 and continuous pasture 11700. Using an initial soil nitrogen value of 0.100% eleven sequences were simulated over a period of 100 years. The sequences were then ranked in order of decreasing soil nitrogen content.

Table 1. Ranking of projected soil organic nitrogen values beginning with an initial soil nitrogen content of 0.100% and running the model for 100 years.

Crop Sequence	Projected Soil nitrogen percentage after 100 years
PP	0.217
WPPP	0.146
WPP	0.129
WWPP	0.118
WP	0.111
WWP	0.101
WWWP	0.091
FWPP	0.085
FWP	0.062
WW	0.059
FW	0.040

Six of the sequences maintained or increased soil nitrogen content. None of the sequences containing fallow were in this category and the most drastic sequence in terms of soil nitrogen loss was FW. The relative low value of continuous wheat is associated with the low yields obtained with this sequence. It is of interest to note the effect of higher crop yields of this sequence as shown by equilibrium soil nitrogen contents i.e. when $dN/dt = 0$. Equilibrium values with wheat dry matter yields of 3000, 4000 and 5000 kg ha^{-1} are 0.062, 0.082 and 0.103% N respectively. This indicates that soil nitrogen levels could be maintained at 0.100% N in a continuous wheat sequence with dry matter yields of 5000 kg ha^{-1}. The sequences WP and WWP slightly increased or maintained soil nitrogen at 0.100% N and given the relatively high rainfall of this station would appear to be satisfactory cropping sequences from the point of view of soil organic nitrogen maintenance and moderate cropping intensity.

FEEDBACK EFFECTS OF SOIL ORGANIC MATTER LEVELS ON CROP AND PASTURE YIELDS

Although the model used to predict the effect of crop and pasture sequences on soil organic matter is useful it does not take into account the effect of soil organic nitrogen on crop yield. Thus as the soil organic nitrogen levels fall the amount of available nitrogen mineralized annually falls and in the absence of applied fertilizer or practices such as fallowing crop yields decline. With declining crop yields the amount of plant residues returned annually also decline and soil organic nitrogen levels continue to fall until a new equilibrium is established.

Lucas et al. (1977) presented a model of soil carbon feedback influences on maize yield response to nitrogen. Their Michigan data indicated that soil equilibrium carbon levels ranged from a low value of 1.1% C (or 0.110% soil organic N assuming a C:N ratio of 10:1) where no additional nitrogen was applied to a value exceeding 3.4% (or 0.340% soil organic N) with intensive nitrogen fertilization. Equivalent maize grain yields in these extremes were 3400 kg ha^{-1} to 11300 kg ha^{-1}. However the authors suggest caution in the interpretation of their projections particularly as the bounds of validity of the soil carbon-yield potential relationship may have been exceeded.

The relative beneficial physical effects of soil organic matter on crop yields as compared with the chemical effects of nutrients released from soil organic matter is likely to differ for different soils. In particular the structural stability of a soil at different organic matter levels is an important consideration. Work at Rothamsted (Boyd, 1967) on soils with relatively high structural stability has shown that yield differences in test crops following pasture leys could be explained almost entirely in nutrient terms and basically this came down to differences in nitrogen. On such soils application of equivalent nitrogen could duplicate effects due to ley. On the other hand on soils with lower structural stability (Greenland, 1971) there appear to be benefits on crop yield associated with increasing soil carbon as distinct from effects due to additional available nitrogen.

MODEL OF THE FEEDBACK EFFECT OF CROP YIELD ON SOIL ORGANIC NITROGEN

Soil organic nitrogen declines are currently occurring on cropped soils in the semi-arid subtropics of eastern Australia (e.g. Martin and Cox, 1956). Many of these soils were originally under natural grassland or forests of the leguminous tree *Acacia harpophylla* (brigalow). Virgin soil organic nitrogen levels were mostly in the range of 0.15-0.25% N but in some soils levels were higher than 0.40%. Little applied nitrogen is used on these soils in the lower rainfall areas at present but as soil nitrogen reserves decline questions arise as to likely equilibrium soil nitrogen levels, the extent to which crop yields will be affected and how changes in crop yield and soil organic matter levels can be influenced by applied nitrogen fertilizer or crop sequences.

Experiments were begun in 1967 at Narayen Research Station (lat. 25°41'S, long 152°52'E) on cropping virgin grey-brown clay soils (vertisols) with grain sorghum (*Sorghum bicolor*) as one of the treatments. This station has an annual rainfall of 713 mm, an annual evaporation of 1840 mm and an annual temperature of 19.7 °C. Rainfall is summer dominant with 59% falling in the period November to March. Crop yields were recorded annually and soil samples were taken biennially. Substantial declines in soil organic nitrogen were found.

To examine relationships between crop yield and soil organic nitrogen change and to project future trends of both as affected by applied nitrogen a model of the form shown in Figure 2 was used.

The equation for soil organic nitrogen in this model was:

$$dN/dt = -K_1N + K_3Y(t) \qquad (4)$$

where the coefficients K_1 and K_3 were similar to equation (3) and Y(t) was the annual dry

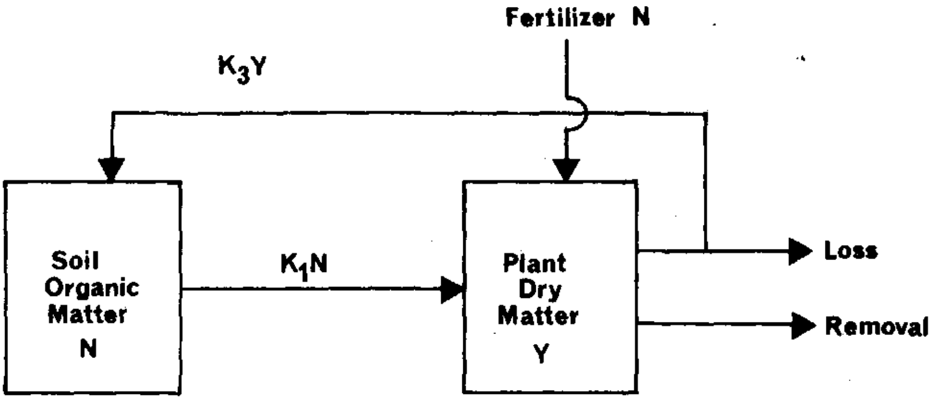


Fig. 2. Diagrammatic representation of the feedback relationship between plant yield and soil organic nitrogen.

matter yield. The effect of nitrogen on crop dry matter yield was expressed as:

$$Y(t) = Y_{max}\,[1-\exp\{-c(K_1N(t) + F(t))\}] \tag{5}$$

In this equation Y_{max} was taken as the maximum crop dry matter yield (kg ha^{-1}) with adequate rainfall and adequate nitrogen and Y(t) was the crop yield as related to soil nitrogen content N(t) and F(t) was the amount of nitrogen added as fertilizer in kg N ha^{-1}. c and K_1 were constants.

Equation (4) was fitted to the soil and sorghum data from Narayen over the 10 year period 1967-1977 where N was soil organic nitrogen of the 0-10 cm horizon and Y(t) was the sorghum above ground dry matter yield in kg ha^{-1}. Soil nitrogen values were initially high (> 0.3% N) in this experiment but in the 10 year period they fell to just above 0.2% N (Fig. 3). Fitted values of the parameters were $K_1 = 0.0492$ percent year^{-1} $K_3 = 4.69 \times 10^{-7}$ percent N ha year^{-1} kg^{-1} (dry matter) and the model accounted for 97.7% of variation about the mean.

For equation (5) the value of Y_{max} was taken as 10000 kg ha^{-1} and c was 0.022. The model was then used to simulate the effect of three different levels of annually applied nitrogen F(t), nil, 50 kg N, 100 kg N on soil organic nitrogen and crop yield levels over a period of 100 years from an initial soil level of 0.30% N.

The projections indicate that soil organic nitrogen levels will decline with continued cropping to sorghum (Fig. 4). In the absence of applied nitrogen maximum sorghum dry matter yields with adequate rainfall should also decline steadily to 4000 kg ha^{-1} after 100 years (Fig. 5). Application of nitrogen of 100 kg N ha^{-1} should maintain crop yields at close to 10000 kg ha^{-1} and with 50 kg N ha^{-1} yields should be maintained above 8000 kg ha^{-1}. However soil organic nitrogen levels will continue to decline to 0.055% N in the absence of applied nitrogen. There is some feedback effect of increased crop yield on soil

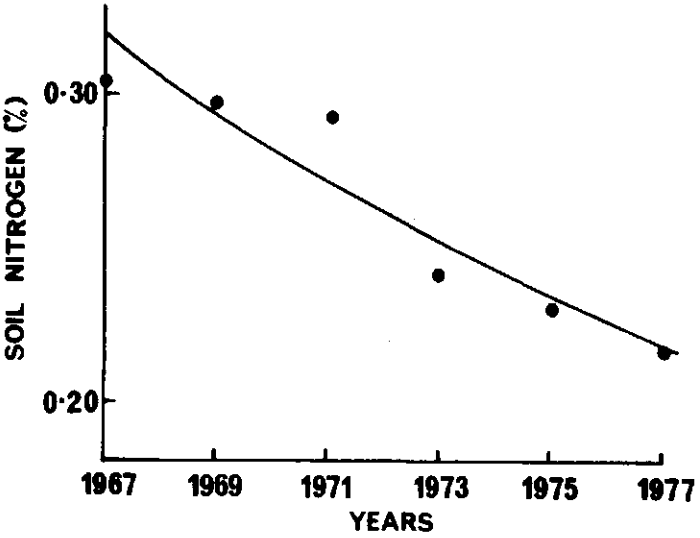


Fig. 3. Changes in the soil nitrogen content of continuous sorghum plots at Narayen Research Station, Queensland, Australia and the estimated changes using the fitted model.

organic nitrogen due to the application of nitrogen fertilizer. If sorghum dry matter yields are maintained at almost 10000 kg ha^{-1} by fertilizer nitrogen the soil nitrogen levels will decline but only to 0.095% N in comparison with 0.055% in the absence of applied nitrogen.

As with any model the projections must be treated with caution. Changes in crop yield have been related entirely to nitrogen and no account has been taken in the model of seasonal differences. These could be expected to produce crop yields lower than the maximum. Although the projected soil nitrogen values appear low, values less than this have been found in soils that have been cropped for many years.

SUMMARY AND CONCLUSIONS

The complexity of the soil organic nitrogen-crop relationships in ecosystems means that modelling has to rely initially on empirical approaches. This places emphasis on the analysis of field situations and the slow rate of change of soil organic matter emphasizes the need for consistent long term data gathering in field experiments. Whilst this does not reduce the need for more fundamental studies of soil organic nitrogen fractions and nitrogen mechanisms it does suggest that much more information on the effects of different soil and climatic parameters on soil organic nitrogen change is required if realistic models are to be developed.

Examples have been given of two simple models using data from two Australian environments. Firstly the effect of crop-pasture sequences has been evaluated using soil and plant

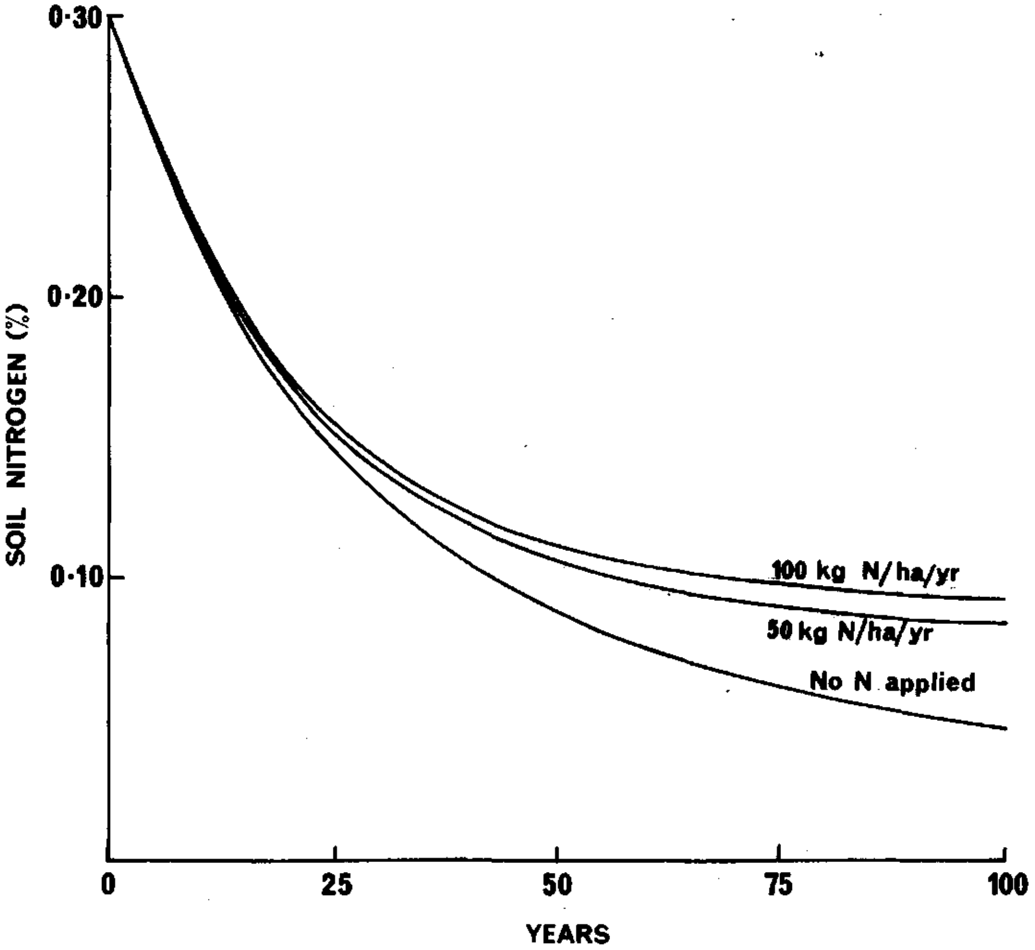


Fig. 4. Simulated change in soil nitrogen content at Narayen with sorghum at three levels of applied nitrogen over a 100 year period.

data from a long-term experiment at the Waite Institute. From the estimated parameters it is possible to project soil nitrogen changes with time and to indicate various combinations of sequences which should maintain soil nitrogen status. Secondly the effect of cropping to sorghum and the feedback effects of crop yield on soil nitrogen levels at Narayen Research Station were studied using soil and plant yield data. This analysis has suggested that soil nitrogen will continue to decline with cropping to lower levels even though crop yields may be maintained by applying nitrogen fertilizer. Feedback effects of increased crop yields due to applied nitrogen on soil nitrogen level is predicted.

A further step in the modelling process would be a combination of both of these approaches in a single model. Thus both the effects of crop-pasture sequences and the feed-

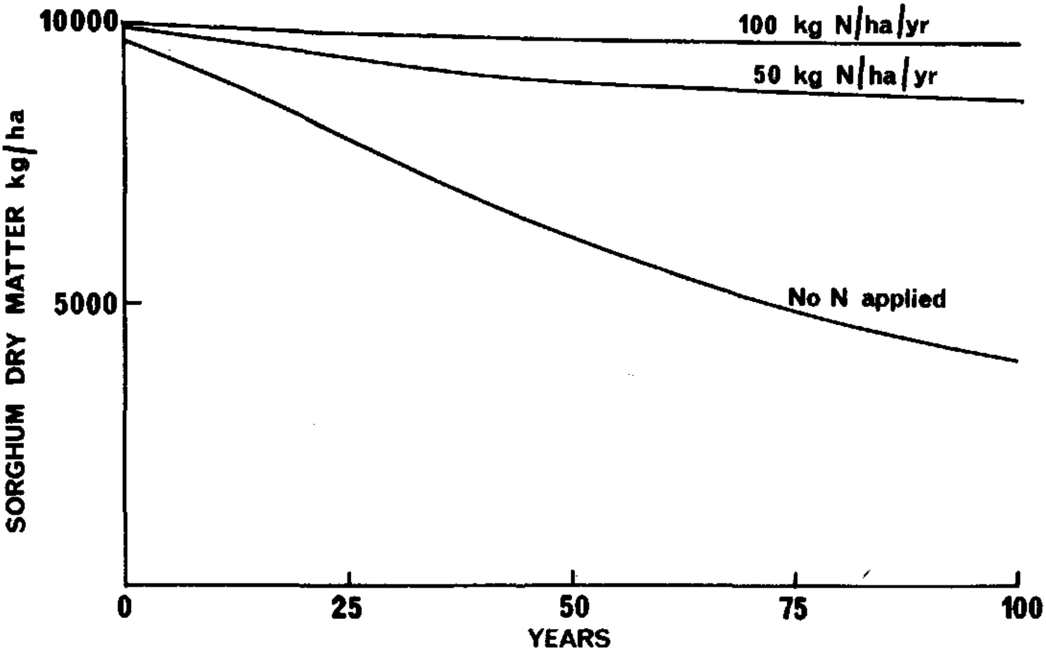


Fig. 5. Simulated change in sorghum dry matter yield at Narayen at three levels of applied nitrogen over a 100 year period.

back effect of crop yields and the effect of applied nitrogen needs to be evaluated but the lack of long term experimental data is a limitation at present to the development of such detailed models. Two areas where further research is necessary are firstly, the identification of easily determined and meaningful soil organic matter fractions useful in field experiments and secondly, definition of land treatment organic nitrogen parameters.

REFERENCES

Bartholomew, W.V., and D. Kirkham, 1960. Mathematical descriptions and interpretations of culture induced soil nitrogen changes. 7th International Congres of Soil Science. Vol. II, 471-477.

Boyd, D.A., 1967. Experiments with ley and arable farming systems. Rothamsted Experimental Station Report, 1967. 316-331.

Clarke, A.L., and J.S. Russell, 1977. Crop Sequential Practices. In: J.S. Russell & E.L. Greacen (Eds): Soil factors in crop production in a semi-arid environment. University of Queensland Press, St. Lucia, p. 277-300.

Dawson, J.E., 1950. In: D.E.H. Frear (Ed): Principles of Agricultural Chemistry. D. van Nostrand, New York, p. 778-797.

Greenland, D.J., 1962. Soil nitrogen changes in the permanent rotation trial at the Waite

Institute. Third Australian Conference of Soil Science. Paper No. 88. Canberra 1962.

Greenland, D.J., 1971. Changes in the nitrogen status and physical condition of soils under pasture with special reference to the maintenance of the fertility of Australian soils used for growing wheat. Soils and Fertilizers 34: 237-251.

Henin, S., G. Monnier, and L. Turc, 1959. Un aspect de la dynamique des matières organiques du sol. Comptes Rendues d'Académie Sciences, Paris 248: 138-141.

Jenkinson, D.S., and J.H. Rayner, 1977. The turnover of soil organic matter in some of the Rothamsted classical experiments. Soil Science 123: 298-305.

Jenny, H., 1941. Factors of Soil Formation. McGraw Hill, New York.

Lucas, R.E., J.B. Holtman, and L.J. Connor, 1977. Soil dynamics and cropping practices. In: W. Lockertz (Ed): Agriculture and Energy. Academic Press, New York, p. 333-351.

Martin, A.E., and J.E. Cox, 1956. Nitrogen studies on black soils from the Darling Downs, Queensland. 1. Seasonal variations and mineral nitrogen fractions. Australian Journal of Agricultural Research 7: 169-183.

Nye, P.H., and D.J. Greenland, 1960. The soil under shifting cultivation. Commonwealth Bureau of Soils Technical Communications. No. 51.

Richardson, H.L., 1938. The nitrogen cycle in grassland soils with especial reference to the Rothamsted Park Grass Experiment. Journal of Agricultural Science 28: 73-121.

Ross, P.J., 1971. A computer program for fitting non linear regression models to data by least squares. CSIRO Division of Soils Technical Paper No. 6.

Ross, P.J., 1973. DIFFEQ - a computer program for continuous system simulation. CSIRO Division of Soils Technical Paper No. 20.

Russell, J.S., 1960. Soil fertility changes in long term experimental plots at Kybybolite, South Australia. 1. Changes in pH, total nitrogen, organic carbon and bulk density. Australian Journal of Agricultural Research 11: 902-926.

Russell, J.S., 1962. Estimation of the time factor in soil organic matter equilibration under pastures. Transactions of the Meetings of Commission IV and V of the International Society of Soil Science. New Zealand, p. 191-197.

Russell, J.S., 1964. Mathematical expression of seasonal changes in soil organic matter. Nature 204: 161-162.

Russell, J.S., 1968. Nitrogen fertilizer and wheat in a semi-arid environment. 2. Climatic factors affecting response. Australian Journal of Experimental and Animal Husbandry 8: 223-231.

Russell, J.S., 1975. A mathematical treatment of the effect of cropping system on soil organic nitrogen in two long term sequential experiments. Soil Science 120: 37-44.

Sims, H.J., 1977. Cultivation and fallowing practices. In: J.S. Russell & E.L. Greacen (Eds.): Soil factors in crop production in a semi-arid environment. University of Queensland Press, St. Lucia, p. 243-261.

Woodruff, C.M., 1949. Estimating the nitrogen delivery of soil from the organic matter determination as reflected by Sanborn field. Soil Science Society of America Proceedings 14: 208-212.

4.12 NH_3 volatilization model

W.J. Parton, W.D. Gould, F.J. Adamsen, S. Torbit and R.G. Woodmansee

1. NAME OF MODEL

NLOS

2. SYSTEM MODELED

The model is designed to simulate the volatilization losses of NH_3 from cattle urine patches. NLOS simulates the transformation and movement of urea in the soil and volatilization of NH_3 from the soil.

3. OBJECTIVE

The primary objective of the model is to better understand the environmental and physical factors which control the volatilization of NH_3 from urine patches. In particular we are interested in the effect of soil temperature, soil texture, pH, evaporation rate, and soil moisture on the NH_3 volatilization losses from a urine patch. It is anticipated that a prediction model for field application will be developed by simplifying the NLOS model.

4. TIME-SCALE

The model is designed to run for time periods up to 14 days using one-minute and five-minute time steps for the fast and slow components of the model. The slow part of the model includes the soil water flow model and the hydrolysis of urea, while the rest of the model runs at the fast time step.

5. DIAGRAM

Figure 1 shows a flow diagram of the model. The major state variables include urea, NH_4^+ in soil solution (NH_4^s), NH_4^+ adsorbed to soil colloids (NH_4^F), NH_3 in soil solution (NH_3^{ag}), and NH_3 gas in soil atmosphere (NH_3^g). The flows include hydrolysis of urea, establishing an equilibrium between NH_4^s and NH_4^F, NH_4^s and NH_3^{ag}, and NH_3^{ag} and NH_3^g, and diffusion of NH_3 gas from the soil. The model was set up for a 5-cm soil core, and the state variables are calculated for each of the 6 soil layers (0 to 0.25 cm, 0.25 to 1 cm, 1 to 2 cm, 2 to 3 cm, 3 to 4 cm, and 4 to 5 cm). The state variables in the model are the amount in each of the compartments (Fig. 1) and are calculated by multiplying the concentration ($g.cm^{-3}$) of each component by the volume of water, soil, or air that it is part of. The model also predicts the flow of water within the soil and evaporation of water at the soil surface. The water flow model considers both saturated and unsaturated water flow. The model distinguishes

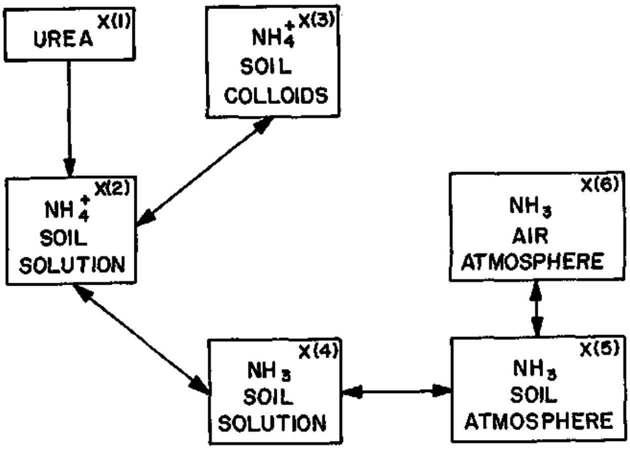


Fig. 1.

between vapor and liquid flow of water and simulates the flow of soluble compounds (NH$_4^s$, urea, and NH$_3^{ag}$) between soil layers. The model also simulates the flow of NH$_3^g$ within the soil.

6. LEVELS

The levels or integrals used in the model are:

a. Nitrogen (g·m^{-2}) for each soil layer

X(1) = Urea

X(2) = NH$_4^+$ in soil solution

X(3) = NH$_4^+$ adsorbed to soil colloids

X(4) = NH$_3$ in soil solution

X(5) = NH$_3$ in soil atmosphere

X(6) = NH$_3$ in the free atmosphere

b. Soil water (cm H$_2$O)

θ_i = Soil water content in the ith soil layers.

7. GOVERNING EQUATIONS

The model includes a nitrogen cycling submodel and water flow submodel. The description of each of the submodels will be organized around the flows, with each of the flows representing a process considered in the model (i.e. hydrolysis of urea).

Hydrolysis of urea

The hydrolysis of urea is calculated as a function of the contentration of urea in the soil (C_V), the soil temperature, and the pH of the soil with the following equations:

$$H = V_M \cdot C_V \cdot M_t \cdot P / (K_M + C_V) \tag{1}$$

where

H = the hydrolysis rate ($\mu g\ N.g^{-1}.sec^{-1}$)
V_M = the maximum rate of hydrolysis ($\mu g\ N.g^{-1}.sec^{-1}$)
K_M = the Michaelis constant ($\mu g\ N.g^{-1}$)
M_t = the effect of soil moisture on hydrolysis
P = the effect of pH on hydrolysis.

V_M increases exponentially as a function of temperature according to the following equation:

$$V_M = A\ e^{(-E_a/RT)} \tag{2}$$

where

T = the soil temperature (^oK)
E_a = the activation energy (9.8 kcal . mole^{-1})
R = a gas constant (1.98×10^{-3} kcal . mole^{-1} . $^oK^{-1}$)
a = an experimentally determined constant ($A = 153980\ \mu g.g^{-1}.sec^{-1}$).

The effect of soil moisture (M_t) and pH (P) on hydolysis are shown in Fig. 2a and 2b, respectively. The flow to soil solution NH_4^+ is calculated by multiplying the hydrolysis rate by the soil concentration of urea using a 300 second time step.

The pH of each soil layer is calculated as function of cumulative hydrolysis of urea (Fig. 3). As ammonia is volatilized the pH will tend to decrease as a result of dissociation of NH_4^+ ion. This effect is included in the model by subtracting the cumulative loss of NH_3 gas ($\mu g\ N.g^{-1}$) for each layer from the cumulative hydrolysis of urea.

Equilibrium between NH_4^s and NH_4^F

The model calculates an equilibrium between NH_4^+ in solution (NH_4^s) and NH_4^+ adsorbed by the soil colloids (NH_4^F).

$$NH_4^s \overset{K_1}{\rightleftarrows} NH_4^F \tag{3}$$

The equilibrium constant K_1 is calculated as a function of solution concentration ($\mu g.ml^{-1}$) of NH_4^+ ((NH_4^s)), according to the following equation:

$$K_1 = D/(D + K_A) \tag{4}$$

$$D = (NH_4^s) + 50 \tag{5}$$

where K_A (20 $\mu g.ml^{-1}$) is the Michaelis coefficient. The model calculates flows such that

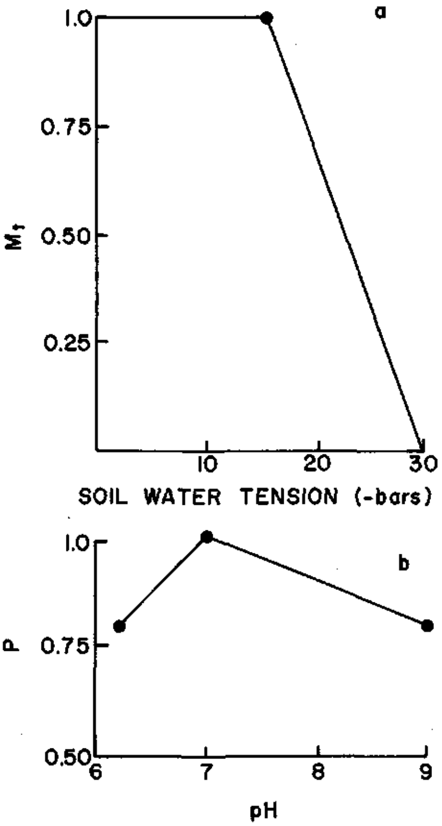


Fig. 2.

the instantaneous equilibrium between NH_4^s and NH_4^F will be established. This series of equations was set up so that the fraction of total NH_4^+ in each soil layer that is adsorbed by soil colloids will increase with solution concentration of NH_4^+. Conceptually, this equation includes the precipitation of salts and other fixation mechanisms in addition to NH_4^+ held by the cation exchange complex. Drying down of the soil is one of the main processes for increasing the solution concentration of NH_4^+ ion. This part of the model uses a 15-second time step.

Equilibrium among NH_4^s, NH_3^{ag}, and NH_3^g

The model uses the chemical equilibrium between NH_4^s and NH_3^{ag} and an equilibrium between NH_3^{ag} and NH_3^g.

$$NH_3^{ag} + H_2O \overset{K_2}{\rightleftarrows} NH_4^s + OH^- \qquad (6)$$

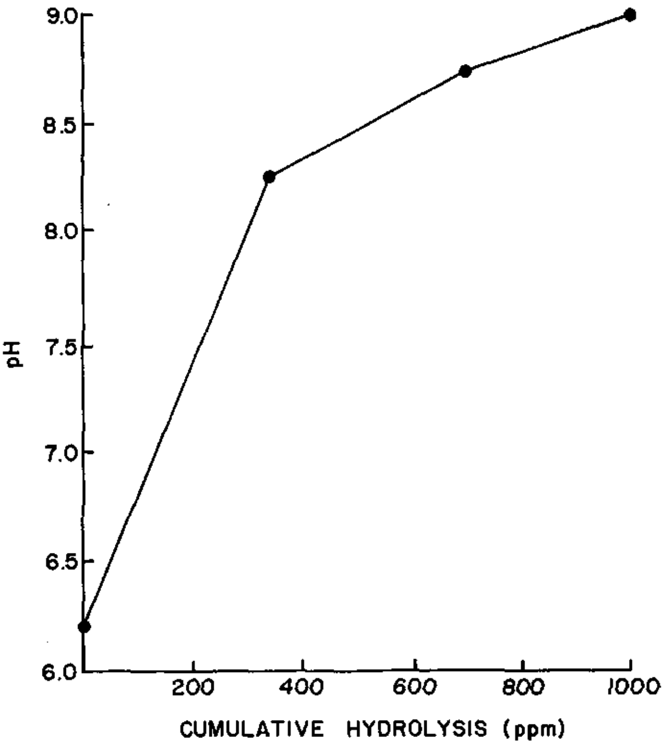


Fig. 3.

$$NH_3^{ag} \overset{K_3}{\rightleftarrows} NH_3^{g} \qquad (7)$$

These equilibriums are solved simultaneously using the following equations:

$$N^T = X(2) + X(4) + X(5) \qquad (8)$$

$$K_2/(OH^-) = (NH_4^s)/(NH_3^{ag}) \qquad (9)$$

$$K_3 = (NH_3^g)/(NH_4^{ag}) \qquad (10)$$

where

N^T = the sum of X(2), X(4), and X(5)
K_2 and K_3 = temperature-dependent equilibrium coefficients (Van Veen, 1977)
(OH^-) = OH^- activity
(NH_4^s) and (NH_3^g) = concentrations (g.cm^{-3} water) of NH_4^s and NH_3^{ag}, respectively and (NH_3^g) is the concentration (g.cm^{-3} air) of NH_3^g.

(OH^-) is calculated as a function of the pH according to the following equation:

$$(OH^-) = 10^{(-14 + pH)} \quad (11)$$

The temperature dependence of this equation is ignored because of its relatively small effect. This part of the model uses a 15-second time step.

Solution transport of urea, NH_4^s, and NH_3^{ag}

Urea, NH_4^s, and NH_3^{ag} are in the soil water solution and are transported between soil layers with liquid water flow. The soil water flow model calculates the water flow between layers, and the fraction of the water flow in the liquid phase is a function of the soil water tension. The fraction of water flow in the liquid phase is equal to 1 with soil water tension greater than -3 bars and decreasing to zero at -15 bars water tension. The solution transport is assumed to equal the liquid water-flux times the solution concentration. A 300-second time step is used to calculate the flow.

Diffusion of NH_3^g

The model calculates the diffusion of NH_3 gas within the soil layers and the loss of NH_3 from the top soil layer into the atmosphere. Diffusion of NH_3 gas within the soil is calculated according to Fick's law of diffusion.

$$F_i = [(NH_3^g)_{i-1} - (NH_3^g)_i] \cdot D / \Delta x \quad (12)$$

where

F_i = the flux of NH_3^g from the ith layer to i-1 soil layer (g $N.cm^{-2}.sec^{-1}$)
D = diffusion rate of NH_3^g in the soil ($cm^2 . sec^{-1}$)
Δx = the distance between soil layers
$(NH_3^g)_{i-1}$ and $(NH_3^g)_i$ = the concentrations ($g.cm^{-3}$ air) of NH_3^g in the soil atmosphere of the i-1 and ith soil layers.

The diffusion rate of NH_3^g in the soil is calculated as a function of the porosity of the soil according to the following equation:

$$D/D_0 = S^{1.33} \quad (13)$$

where

S = the fraction of a soil layer occupied by air
D_0 = the diffusion coefficient of NH_3 gas in free air ($0.185\ cm^2 . sec^{-1}$).

This equation was developed by Millington (1959) and the value of D_0 is based on the value used by Van Veen (1977).

Transfer of NH_3^g from the top soil layer to the atmosphere is calculated with the following equation:

$$F^a = [(NH_3^g)_{air} - (NH_3^g)_1] / \gamma \qquad (14)$$

where

F^a = the flux of NH_3^a from the top soil layer into the atmosphere
γ = the resistance to flow of NH_3^g into the atmosphere
$(NH_3^g)_{air}$ and $(NH_3^g)_1$ = the concentration ($g.cm^{-3}$ air) of NH_3^g in the free air and the soil atmosphere of the top soil layer.

γ is a function of wind speed, increasing rapidly with low wind speeds. We assume that wind speed is high enough to break up the boundary layer and is set equal to 0.4 $sec.cm^{-1}$. At the present time the model only considers situations where NH_3^g flows out of the soil. This assumption is valid as we are considering the volatilization of NH_3^g from urine patches where large amounts of urea are added. Diffusion of NH_3^g in soil is simulated using a 15-second time step.

Soil water model

The water flow submodel considers both saturated and unsaturated water flow. The saturated water flow occurs immediately after the application of water to the soil. With the saturated water flow, water is added to the top soil layer until it reaches the -.10 bar water tension. Water not used to fill up the top soil layer is then used to fill up the next lower soil layer until all of the water is allocated. Unsaturated water flow occurs at water tension less than -.10 bars and is calculated with the equation suggested by Hillel (1977). He combined Darcy's law and continuity equation to get the following equation for the vertical flow of water in the soil:

$$\frac{\delta\theta}{\delta T} = \frac{\delta}{\delta Z} (K \frac{\delta\psi}{\delta Z}) - \frac{\delta K}{\delta Z} \qquad (15)$$

where

θ = the soil water content (cm H_2O)
Z = the soil depth
K = hydrolic conductivity ($cm.sec^{-1}$)
ψ = soil water potential (cm water).

This equation is solved with the same finite difference scheme and boundary conditions used by Hillel (1977). The boundary condition at the soil-air interface is that water loss by evaporation equals the potential evaporation rate until the top soil layer reaches the air-dry value of the soil (-50 bar water tension) and is then set equal to the rate that water flows into the top soil layer from the next lower layer. Water loss from the bottom of the soil profile is assumed to equal zero because of our present experimental conditions. The potential evaporation rate is a function of the air temperature and wind speed and is assumed to be constant for any given model run. A 300-second time step is used in solving the water flow model.

8. INPUT PARAMETERS

a. Initial values of N state variables:
1. initial levels of NH_4^s, NH_4^F and urea in each of the soil layers,
2. concentration of urea in the added soil water.

b. Initial condition for the soil water model:
1. initial soil water content of each soil layer (cm H_2O),
2. added soil water (cm of H_2O).

c. Constants for the N model:
1. equilibrium constants for equations (6) and (7) Van Veen, 1977),
2. Michaelis coefficient for equations (4) and (5),
3. diffusion coefficient of gaseous NH_3 ($cm^2.sec^{-1}$) in the soil (equation (11)) and resistance to flow of NH_3 gaseous ($sec. cm^{-1}$) in the free atmosphere,
4. value for K_m and A used in equations (1) and (2) respectively,
5. pH of the soil as a function of cumulative hydrolysis.

d. Constants for the water flow model:
1. relationship of matric potential (cm of head) to volumeter soil water content for each soil layer,
2. relationship of hydrolic conductivity ($cm.sec^{-1}$) to matric potential (cm of head) for each soil layer,
3. depth of each soil layer (cm).

e. Driving variables:
1. soil and air temperature (°C),
2. maximum evaporation rate ($cm.sec^{-1}$).

9. OUTPUT, VERIFIABLE VARIABLES

The main output variables which can be determined by experimental determination are:

a. total NH_4^+ (NH_4^s + NH_4^F) on each soil layer ($g.m^{-2}$),

b. urea N in each soil layer ($g.m^{-2}$),

c. NH_3 loss ($g.sec^{-1}$) vs time and cumulation NH_3 loss ($g.m^{-2}$),

c. soil water content on each soil layer (cm H_2O).

10. OBSERVATIONS

The experiments that were used to determine parameters for NLOS included: an experimental determination of the coefficients used in the urea hydrolysis equations (1 and 2), determination of the relationship between pH of the soil and cumulative hydrolysis of urea,

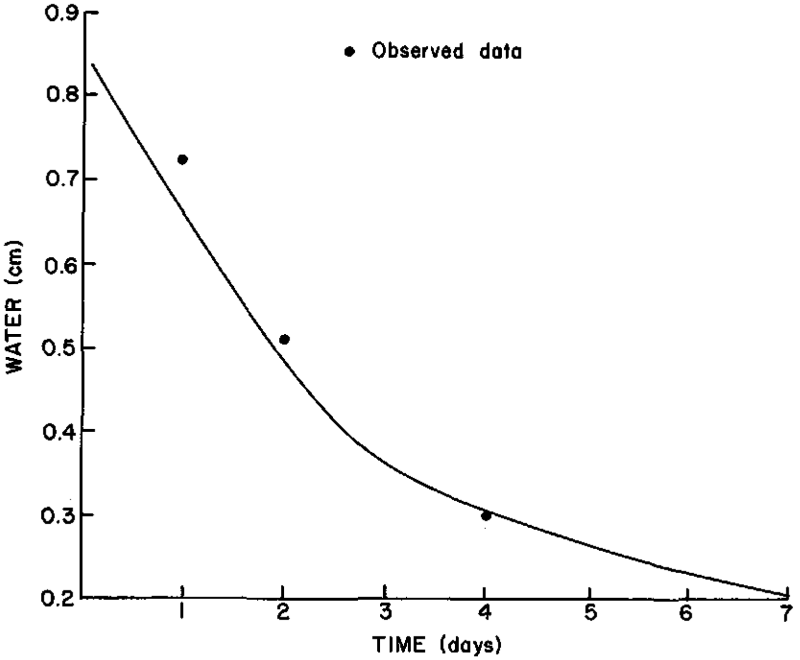


Fig. 4.

and the laboratory determination of the relationship between soil matric potential and soil water content.

Urea hydrolysis rates were measured by the procedure used by Gould et al. (1973), in order to determine the value of V_M in equation (1). The constant A is calculated by inserting the observed value of V_M at 25 °C into equation (2). The effect of temperature (equation (2)) was taken from literature data (Gould et al., 1973). One of the implicit assumptions is that the urease level in the soil remains constant.

The change in the soil pH resulting from urea hydrolysis (see Fig. 3) is determined from an experiment where urea was added to the soil and the change of pH as function of cumulative urea hydrolysis was recorded.

The relationship of soil matric potential and soil water content was determined using standard pressure plate techniques, and the relationship of hydrolic conductivity to matric potential are based on data published by Hillel (1977) for a sandy soil.

11. COMPARISON RESULTS

A detailed verification and validation of the model has not been performed at the present time. Preliminary verification of water flow model has been performed and is presented in Fig. 4. The results show the model does a good job of representing the change in soil water content vs time. It is important to note that observed soil water data was partially used in development of the water flow model. A similar verification of nitrogen cycling part of the model has not been performed at the present time. Figure 5 shows the results

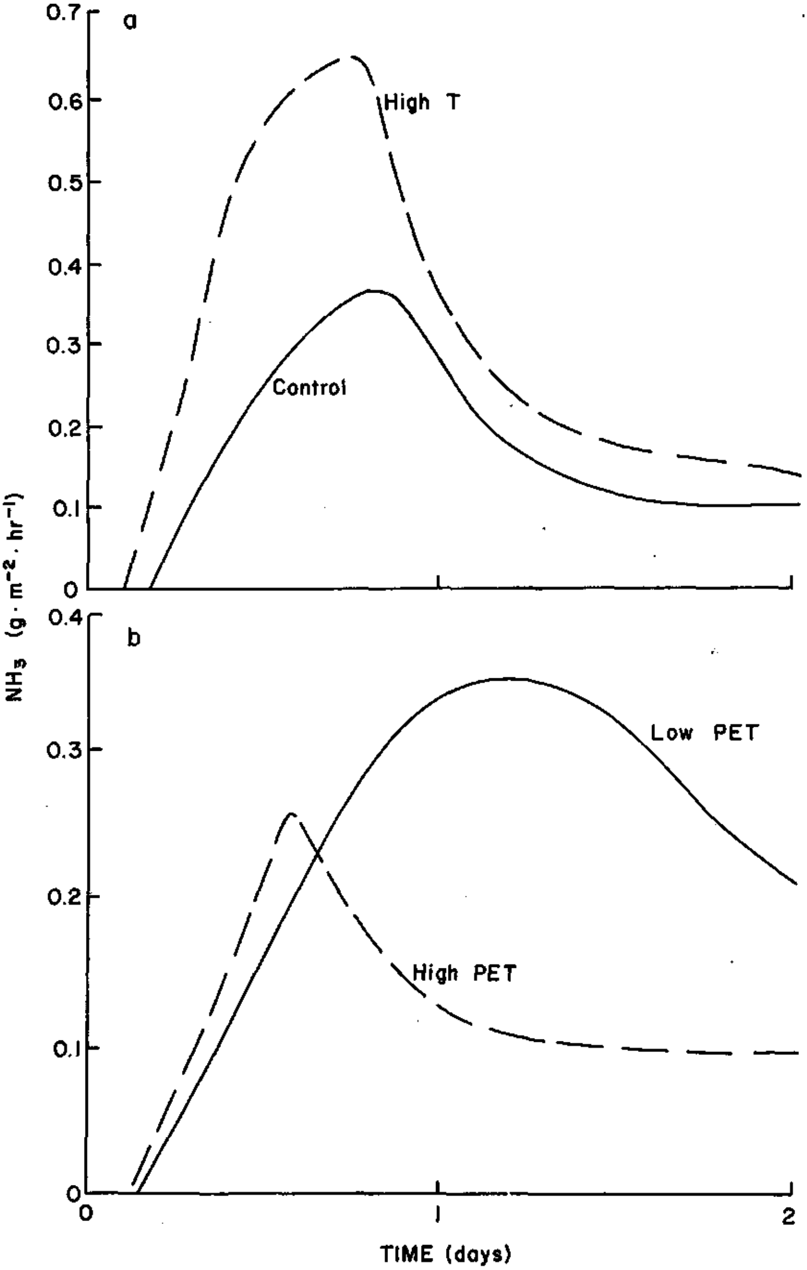


Fig. 5.

of series of model runs where the driving variables for the model have been varied. With the control run the potential evaporation rate (PET) is .25 cm day^{-1} and the temperature is 25 °C. The results show that NH$_3$ volatilization rate increased rapidly to a peak value after 18 hours and then decreased rapidly. Increasing the temperature without modifying the evaporation rate (high T run) causes NH_3 volatilization to be increased substantially and the peak loss rate occurred 2 hours earlier. Decreasing the PET rate to .15 cm day^{-1} causes the peak NH_3 loss rate to be delayed by 12 hours and the decline after the peak is slower than the control run. Increasing the PET rate to .35 cm day^{-1} causes the NH_3 loss rates to be greatly reduced and the time of the peak loss rate is 6 hours earlier than the control. The percentage of added N that is lost through NH_3 volatilization after 48 hours for the different runs are 14%, 20%, 7% and 18% respectively for the control, high temperature, high PET and low PET runs.

The only observed data we have is volatilization of NH_3 from urine added to a different soil type. With this experiment the temperature was 25 °C and maximum evaporation rate is unknown. The results show that the time of the peak NH_3 loss rate is similar to the control run and that the peak NH_3 losses are 4 times smaller than the control run.

12. LIMITS AND LIMITATIONS

There are no particular limitations to the NLOS model other than the fact that the NH_3 volatilization part of the model has not been validated adequately. Within the next six months we hope to have sufficient experimental data to validate the model.

13. COMPUTER

NLOS is running on a CDC cyber computer at Colorado State University.

14. PROGRAM LANGUAGE

The program uses a fortran based simulation compiler (Simcom 4) which is only available at Colorado State University.

15. RUNNING TIME/COST

The program takes 40 seconds CPU time to run a two day simulation and the approximate cost is $6.00 a minute for CPU time.

16. USERS

The model is being developed and used by a NSF supported nitrogen cycling project at Colorado State University.

17. DEVELOPER AND PRINCIPAL CONTACT

The authors of this paper are the developers of the model.

REFERENCES

Gould, W.D., F.D. Cook, & G.R. Webster, 1973. Factors affecting urea hydrolysis in several Alberta soils. Plant and Soil 38: 393-401.

Hillel, D., 1977. Computer simulation of soil water dynamics: A compendium of recent work, Ottawa, IDRC. Box 8500, Ottawa, Canada, 214 pp.

Millington, R.J., 1959. Gas diffusion in porous media. Science 130: 100-102.

Van Veen, J.A., 1977. The behavior of nitrogen in soil; a computer simulation model. Ph.D. Thesis. Vrije Universiteit, Amsterdam, 164 pp.

4.13 Leaching of nitrate in structured soils

T.M. Addiscott

1. NAMES OF MODELS (AND PROGRAMS)

SL3, SLD3.

2. SYSTEM MODELLED

Leaching of nitrate on plot or field scale in structured soils, mainly to 0.5-1.0 m depth, occasionally to ca. 30 m.

3. OBJECTIVE

Simulation of downward movement or loss of nitrate and other non-adsorbed solutes to give predictions of solute concentrations in the profile and in drainage. The model is particularly intended to make allowance for the holding back of solute in structural units.

4. TIME SCALE

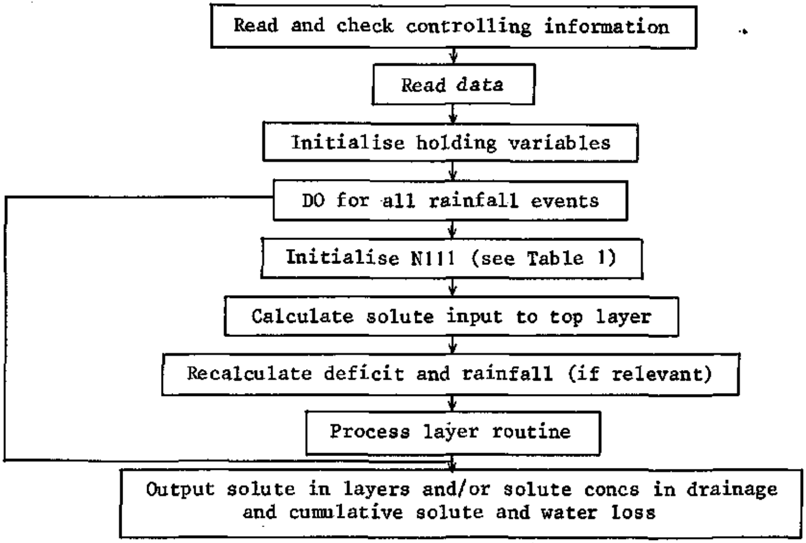
(a) For simulations in shallow profiles (up to 1 m), the total period is usually 3-8 months with computations made once per day when rain occurs.

(b) For simulations in deep profiles (e.g. 30 m) simulations have been made over an 18-year period, with computations once per month.

5. DIAGRAM

This is a layer model based on the concept that water and solutes in the soil can be partitioned between a mobile and a retained phase. There are therefore two compartments per layer and usually between 5 and 30 layers. During water movement, only the mobile phase is displaced. In the simpler model (SL3), it is assumed that equilibrium is set up between the mobile and retained phases when flow ceases. In the SLD3 model, solute moves between the phases by diffusion when flow ceases. Solute in the retained phase is held back against leaching in both instances.

Fig. 1 shows an outline flow chart applicable to both models and table 1 lists the meanings of the variables to which reference is made. The simple calculations that are made for the mobile phase of each layer are shown diagrammatically in Fig. 2a. If the amount of displacement caused by rain (W) exceeds the amount of water in the mobile phase (WM_i), the model follows the fast leaching routine (Fig. 2b and section 7) in which it tests through how many layers the mobile solution is displaced by summing the values of WM_i downwards until $\Sigma WM_i > W$. The mobile solute ΣSM_i for the layers for which $W > \Sigma WM_i$ is stored in



Layer routine

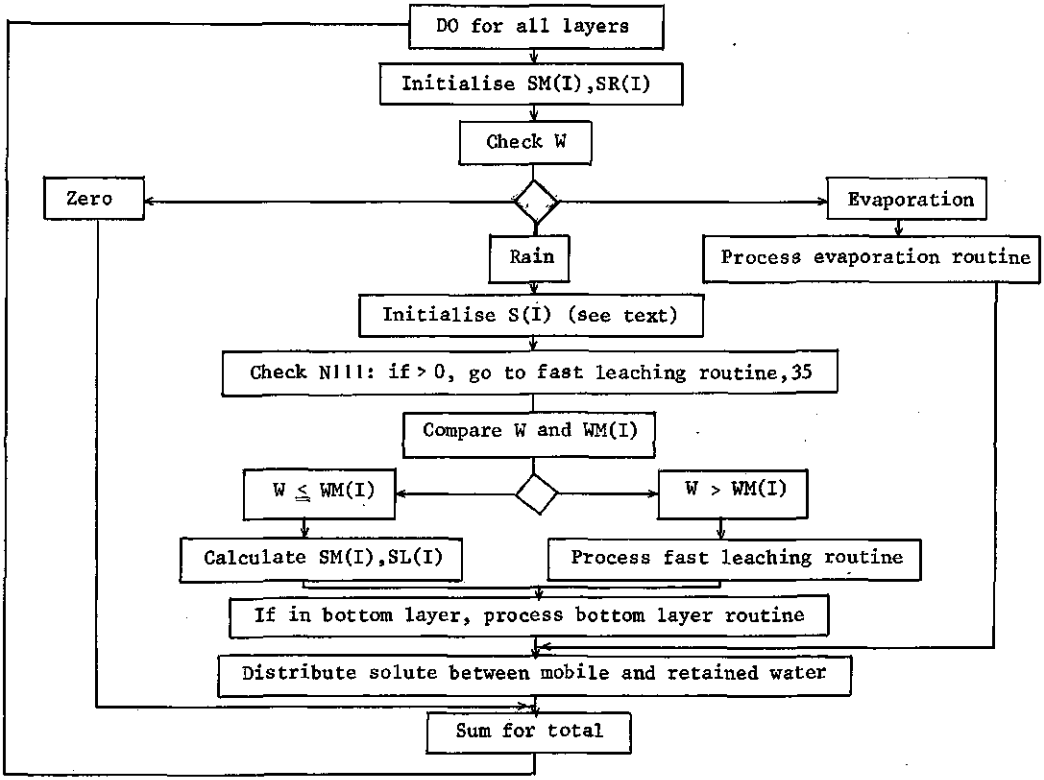


Fig. 1. Outline flow chart applicable to SL3 and SLD3 (Addiscott, 1977).

Table 1. Meanings of variables

WM(I)	Mobile water in layer (I)
WR(I)	Retained water in layer (I)
SM(I)	Solute in WM(I)
SR(I)	Solute in WR(I)
W	Rainfall input
S(I)	Solute input to I'th layer
SL(I)	Solute loss from I'th layer
N111	Layer count for fast leaching routine. Number of layers for which $W > \Sigma$ WM(I)
WN	Σ WM(I) as above
IX	Layer at which W found to exceed WM(I)
IY	Variable
SMC, WMC	Solute and water displaced from layers for which $W > \Sigma$ WM(I)
M	Number of bottom layer
MX1, MX2, MX3	Layers at which it is required to interrupt the fast leaching routine

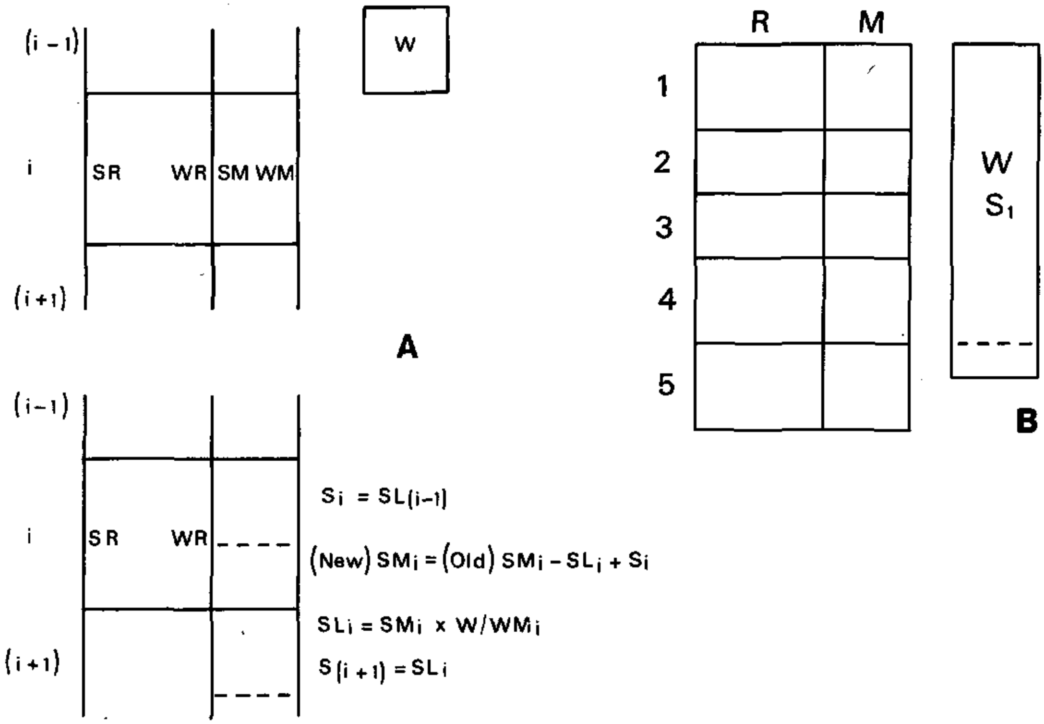


Fig. 2. Diagrammatic representation of calculations made in program. (a) When W < WM(I); (b) When W > (WM(I)).

the layer at which $\Sigma\ WM_i > W$. The solute input (S_i) to the original layer is then distributed between these layers according to their WM_i values (Fig. 2b) and the stored solute distributed subsequently in the layers below.

Evaporation can be accumulated at the surface as a deficit and subtracted from rainfall or treated as 'negative rainfall'.

In the SL3 model the equilibration between the phases after flow ceases is achieved simply by making SM_i/WM_i equal to SR_i/WR_i (Fig. 2a). In the SLD3 model, the movement of the solute between the phases by diffusion requires that the phases have definite sizes and geometry. It is assumed that the retained water is held inside the soil structural units, which are assumed to be cubic, and that the mobile water flows in a film over the surfaces of the cube. Each cube is divided into four concentric volumes (Fig. 3) for each of which the surface area (A) can be calculated. The solute, which is a variable, and the volume of water, which is treated as constant and calculated from the total volume and porosity of the cube. The diffusive flux of solute is then calculated by applying Fick's law in its basic form (see 7).

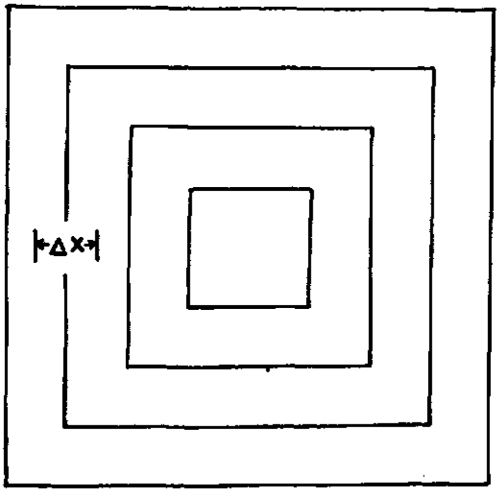


Fig. 3. Two-dimensional representations of the concentric volumes in the cube. (Three-dimensional in model).

6. LEVELS

The levels are in effect the compartments (see 5) and there are no integrations.

7. GOVERNING EQUATIONS

For solute movement between layers in mobile phase, see 5, especially Fig. 2a. The operation of the fast leaching routine is not easily expressed other than verbally (see 5) or in Fortran:

Fast leaching routine

```
1   WN=WM(I)
    IX=I
    IY=I
    IF(I.EQ.M.OR.I.EQ.MX1.OR.EQ.MX2.OR.I.EQ.MX3)GO TO 34
31  IY=IY+1
    N111=N111+1
    WN=WN+WM(IY)
    IF(W.GT.WN)GO TO 32
    GO TO 34
32  IF(IY.EQ.M.OR.IY.EQ.MX1.OR.IY.EQ.MX2.OR.IY.EQ.MX3)GO TO 33
    GO TO 31
33  N111=N111+1
34  SMC=0.0
    WMC=0.0
35  SMC=SMC+SM(I)
    WMC=WMC+WM(I)
    SL(I)=SMC+S(IX)*(W-WMC)/W
    SM(I)=S(IX)*WM(I)/W
    N111=N111-1
    GO TO 4
```

The diffusion of solute between the mobile solution and the outermost volume of the cube and between the concentric volumes within the cube is treated by Fick's First Law

$$F = -D \frac{dc}{dx} \qquad (1)$$

used in the following form, derived from eq. 4.15 of Nye and Tinker (1977)

$$\frac{1}{A}\frac{\Delta S}{\Delta t} = - D_1 \ \theta \ f_1 \frac{\Delta C_1}{\Delta x} \qquad (2)$$

where

A = surface area (mm^2) (see 5)
$\Delta S/\Delta t$ = solute transfer per unit time (mg d^{-1} or mg $month^{-1}$)
D_1 = diffusion coefficient in free solution (mm^2 d^{-1} or mm^2 $month^{-1}$)
θ = volume fraction of water (which gives the cross section for diffusion through solution)
f_1 = impedance factor (which takes account of tortuosity)
$\Delta C_1/\Delta x$ = concentration gradient in liquid phase (mg mm^{-3}).

D_1 is known; A, θ and ΔC_1 are calculated from other inputs; f_1 is assumed to be similar in value to θ; Δx is shown in Fig. 3. The model allows diffusion to take place in any number of time steps.

8. INPUT PARAMETERS

Both models: rainfall and evaporation (mm), solute concentration in rainfall (mg l^{-1}), initial solute concentrations in water in layers (mg l^{-1}), bulk density of soil for some conversions. SL3: soil moisture characteristics for layers from which the values of WM and WR are calculated thus:

$$WM = [\theta(\mathrm{pF}\ 1.7) - \theta(\mathrm{pF}\ 3.3)].d \qquad (\mathrm{mm}) \tag{3a}$$

$$WR = [\theta(\mathrm{pF}\ 3.3) - \tfrac{1}{2}\theta(\mathrm{pF}\ 4.2)].d \qquad (\mathrm{mm}) \tag{3b}$$

where

θ = volume fraction of water
d = layer thickness (mm).

SLD3: aggregate size distributions for layers (normal or log-normal) expressed as mean and standard deviation. (From these the model devides the aggregates into four size categories, each containing one quarter of the volume and derives a mean size for the category. Separate diffusion calculations are subsequently made for each size category.) Porosity of aggregates. Thickness of film of mobile water. (Not measurable; 'guesstimate' needed.)

Note: Nitrate released by mineralisation of soil organic nitrogen has been fed into both programs. Experiments have shown that the amount mineralised is often related to the square root of time by a constant (k) (Stanford & Smith), 1972) and that ln k is proportional to the reciprocal of the absolute temperature (Stanford et al., 1973). These relationships have been used.

9. OUPUT; VERIFIABLE VARIABLES

(a) Amount or concentration of solute in water in each layer (can be converted to dry soil basis).
(b) Concentrations of solute in drainage resulting from each rainfall event.

10. OBSERVATIONS

(a) Small field experiment, not intended for testing of models, in which calcium nitrate was applied to the surface of the soil or incorporated to a depth of 13 cm in early October. 0-13 cm and 13-26 cm layers sampled until mid-January.
(b) Experiment in which chloride was applied in mid-October to the 20-inch and 40-inch (approx. 0.5 and 1.0 m) Drain Gauges (lysimeters) at Rothamsted. Drainage collected daily until the end of May and analysed for Cl.

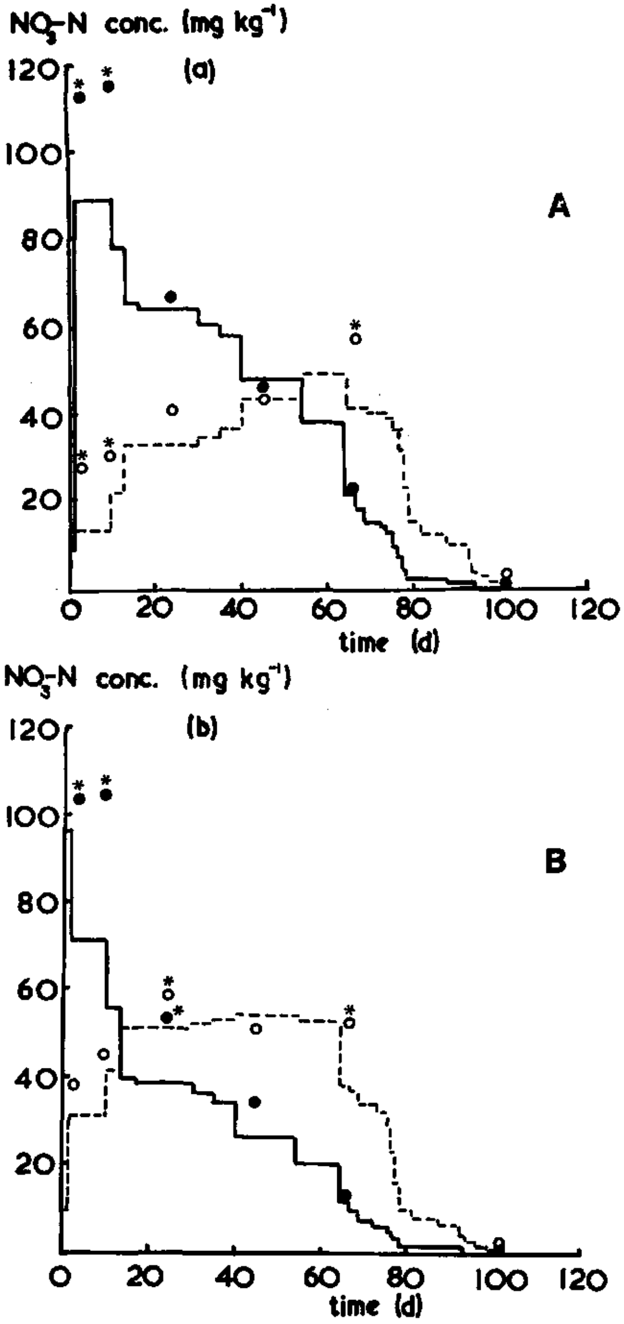


Fig. 4. Measured (points) and simulated (lines) NO_3-N concentrations (dry soil basis) found during experiment described in section 10(a) in 0-13 cm (—— ●) and 13-26 cm (---- o) layers after (a) surface application or (b) incorporation of $Ca(NO_3)$ at 100 kg N ha^{-1}. Asterisk denotes that simulation was outside fiducial limits ($p < 0.05$) of measured concentration (from Addiscott (1977)).

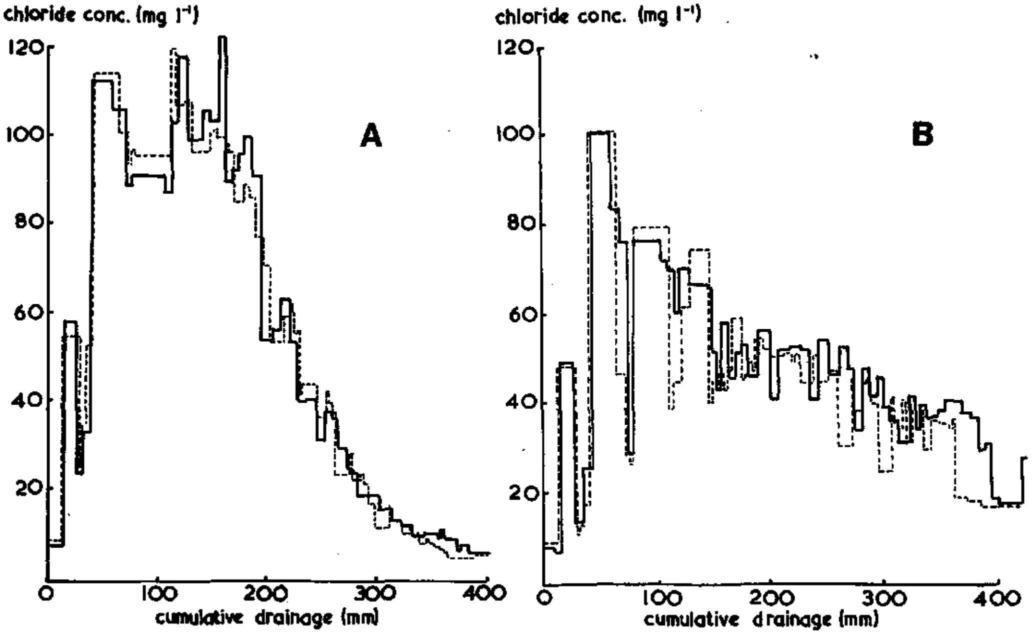


Fig. 5. Relationship between chloride concentration and cumulative drainage in Rothamsted Drain Gauge experiment (section 10(b)). (a) 20-inch, (b) 40-inch gauge. —— measured, --- simulated. (Measured line as in Addiscott et al. (1978), simulation obtained subsequently.)

11. COMPARISON RESULTS

Fig. 4 shows the simulation of the results of the field experiment (10a) and Figs. 5a and b the simulations of the chloride concentrations in the drainage from the Drain Gauges (10b).

12. LIMITS AND LIMITATIONS

When rainfall is put in on a daily basis a layer thickness of 50 mm is appropriate. If monthly inputs are used the layer thickness must also be increased, to 500 or 1000 mm.

The models are intended mainly for structured soils and may not be so relevant in sandy soils, where the model of Burns (1974) may be more appropriate.

13. COMPUTER

The models have both been run in the Rothamsted ICL 470/472 system. SL3 has also been run in a Commodore Pet 8000 microprocessor.

14. PROGRAMME LANGUAGE

FORTRAN.

15. RUNNING TIME/COST

SL3. For a 10 layer profile and 150 rainfall/evaporation events 1 ETU.

SLD3. For a 31 layer profile and 207 rainfall/evaporation events 34 ETU.

16. USERS

Model used so far only at Rothamsted.

17. DEVELOPER AND PRINCIPAL CONTACT

Dr. T.M. Addiscott
Rothamsted Experimental Station
Harpenden
Herts. AL5 2JQ
U.K.

REFERENCES

Addiscott, T.M., 1977. A simple computer model for leaching in structured soils. Journal of Soil Science 28: 554-563.

Addiscott, T.M., D.A. Rose, & J. Bolton, 1978. Chloride leaching in the Rothamsted Drain Gauges: Influence of rainfall pattern and soil structure. Journal of Soil Science 29: 305-314.

Burns, I.G., 1974. A model for predicting the redistribution of salts applied to fallow soils after excess rainfall or evaporation. Journal of Soil Science 25: 165-178.

Nye, P.H., & P.B. Tinker, 1977. Solute movement in the soil-root system. Blackwell, 342 p.

Stanford, G., & S.J. Smith, 1972. Nitrogen mineralisation potentials of soils. Soil Science Society of America Proceedings 36: 465-472.

Stanford, G., M.H. Frere, & D.H. Schwaninger, 1973. Temperature coefficients of soil nitrogen mineralization. Soil Science 115: 321-323.

4.14 A model to simulate partial anaerobiosis

P.A. Leffelaar

1. NAME OF MODEL

ANAER: Partial anaerobiosis in a model soil.

2. SYSTEM MODELED

A structured agricultural soil is represented by spherical porous equidimensional aggregates in a hexagonal packing with inscribed porous aggregates in its voids. For this geometry water and oxygen transport properties are modeled for the top 25 cm of the model soil in view of denitrification.

3. OBJECTIVE

To develop a mathematical approach to the problem of calculating partial anaerobiosis in structured soils taking into account the inter- and intra-aggregate water distribution, the oxygen transport from the atmosphere into the soil and from the inter-aggregate pores into the aggregates. Further to indicate deficiencies in the description of these processes in view of future research.

4. TIME SCALE

The model has been used to calculate the anaerobic soil volume before, during and after short rain periods. Total simulated time is one day and the time step used was 10^{-4} day.

5. DIAGRAM

ANAER is a model composed of the submodels water flow, macro diffusion of oxygen from the atmosphere into the soil, and oxygen diffusion from inter-aggregate pores into the aggregates. In the following the main processes are described.

Water flow: from functions relating water content to suction and hydraulic conductivity respectively, water flows are calculated following Darcy's law and subsequently used to calculate the new water content in each layer. The water flow submodel is based on a paper by Van Keulen & Van Beek (1971). Rain is introduced as a forcing function. Water uptake by roots is assumed to be homogeneously distributed over the profile. The ground water table is situated at a depth of 50 or 100 cm.

Macro oxygen diffusion: from a function relating diffusion efficiency to gas-filled porosity and from mass transport of oxygen out of the profile due to air displacement by rain water, oxygen flows are calculated and used to compute the new oxygen concentration in each layer.

Oxygen diffusion from inter-aggregate pores into the aggregates: functions relating water content to air-exposed area for each aggregate diameter, and to the equivalent radius of the water filled part of an aggregate were calculated. Diffusion of oxygen is taken proportional to air-exposed area, and the equivalent radius is used to compute its ratio to the critical radius at which just no anaerobiosis occurs. This ratio is used in the steady state solution to the diffusion equation for spheres to obtain the anaerobic aggregate volume (Currie, 1961). Respiratory activity is reduced in proportion to the anaerobic soil volume fraction.

6. LEVELS

See 5.

7. GOVERNING EQUATIONS

The equations describing the processes mentioned have previously been derived (Leffelaar, 1977, 1979). The interested reader is referred to the original texts.

8. INPUT PARAMETERS

a. *General inputs*

- radius of equidimensional aggregates, cm
- total pore volume, $cm^3.cm^{-3}$
- total depth of top layer, cm
- number of compartments.

b. *Water flow model*

- initial water contents, $cm^3.cm^{-3}$
- soil moisture characteristic
- hydraulic conductivity as a function of water content (calculated according Green and Corey, 1971)
- saturated hydraulic conductivity, $cm.d^{-1}$
- root water uptake, $cm.d^{-1}$
- depth of groundwater table, cm
- rainfall onset, intensity and duration as a function of time, d.

c. *Oxygen flow model for transport of oxygen from the atmosphere into the soil*

- diffusion efficiency factor as a function of gas-filled porosity (calculated according Millington and Shearer, 1971)
- diffusion coefficient of oxygen in air, $cm^2. d^{-1}$
- amount of oxygen in air, g $O_2.cm^{-3}$
- oxygen consumption rate at the moment that no anaerobic zones are present, g $O_2.cm^{-2}.25$ cm $depth^{-1}.d^{-1}$

d. *Oxygen diffusion from inter-aggregate pores into the aggregates*

- air exposed area as a function of water content for each aggregate diameter
- equivalent radius of the water filled part of an aggregate as a function of water content
- anaerobic soil volume fraction as a function of the ratio of the equivalent radius to the critical radius (calculated according Currie, 1961)
- distribution of the oxygen consumption over the aggregates
- diffusion coefficient of oxygen in pure water, $cm^2 . d^{-1}$
- diffusion coefficient of oxygen in an aggregate, $cm^2 . d^{-1}$ (calculated according Millington and Shearer, 1971)
- critical oxygen concentration at which it is stated that anaerobiosis occurs, g $O_2 . cm^{-3}$
- relative solubility of oxygen in water.

9. OUTPUT; VERIFIABLE VARIABLES

- Anaerobic soil fraction as a function of time.
- Anaerobic aggregate fraction for each aggregate diameter.
- Oxygen concentration in the inter-aggregate pores.
- Water content.

10. OBSERVATIONS

The model was used to indicate which problems need more attention by performing a sensitivity analysis of the different variables, it was not tested experimentally.

11. COMPARISON RESULTS

Results are shown in Figs. 1 through 4, in terms of the fractional anaerobic volume of soil (FANVOL) plotted against time for soil layers 1, 7 and 15 corresponding to average depths of 0.8, 10.6 and 23.7 cm, respectively. The diffusion coefficient in the aggregates, and the rain intensity and duration were taken as 0.1272 $cm^2 . d^{-1}$ and 9 $cm . d^{-1}$ and 3 hours, respectively.

Figure 1 serves as a so-called basic run in which input data for oxygen consumption rate and groundwater depth were taken 10 l $O_2 . m^{-2}$. 25 cm $depth^{-1} . d^{-1}$ and 100 cm, respectively. Input data used to produce Figs. 2, 3 and 4 have been changed as compared to those in Fig. 1 with respect to either oxygen consumption rate (26.7 l $O_2 . m^{-2}$. 25 cm $depth^{-1} . d^{-1}$), or spatial distribution of the respiratory activity, or groundwater depth (50 cm), respectively. Before rain is introduced, about 0.05 day is needed to adjust FANVOL to its right initial value. It is seen that below a depth of 10 cm always some anaerobic microsites are present indicating the soil to be a potential source of denitrification. Further a rain of 11 mm has a pronounced effect on anaerobiosis even up to about 20 hours after it ceases.

A more detailed discussion is given by Leffelaar (1979).

12. LIMITS AND LIMITATIONS

- Maximum time step equals 10^{-4} day, caused by the small time constant of the macro oxygen diffusion process.

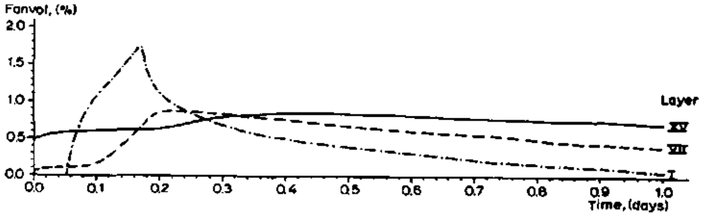


Fig. 1.

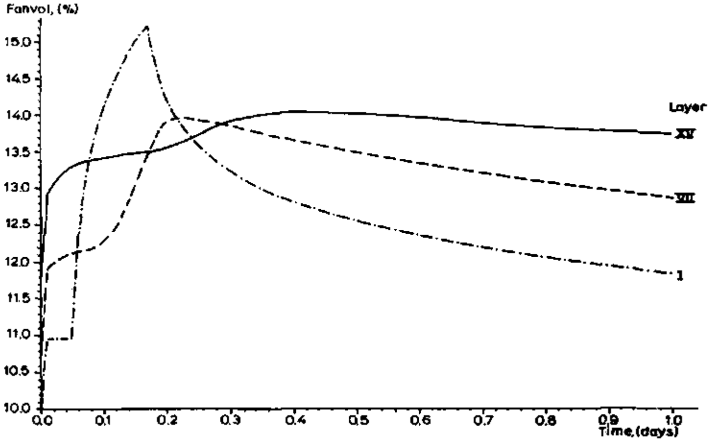


Fig. 2.

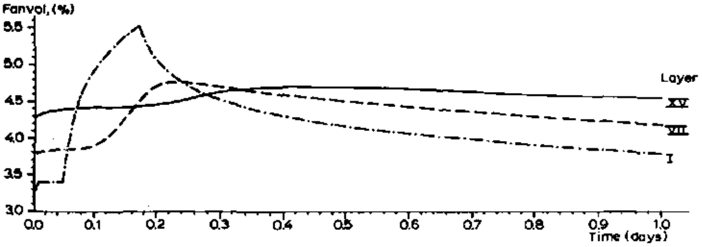


Fig. 3.

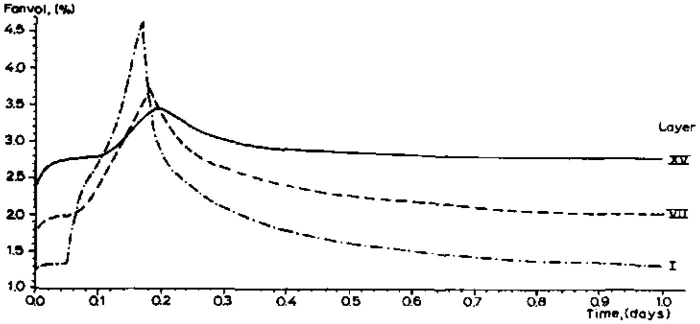


Fig. 4.

Figs. 1-4. FANVOL as a function of time for three layers. From top to bottom 1: basic program, run 1; 2: oxygen consumption 26.7 l $O_2.m^{-2}$. 25 cm $depth^{-1}.d^{-1}$, run 2; 3: respiratory activity located in half the aggregates, run 3; 4: depth of groundwater table 50 cm, run 4. (Figs 1,2 and 4 from: Soil Science 128:110-120.Williams & Wilkins Co.Baltimore,USA)

- Space steps were taken as the height of a unit hexagonal packing. When the diameter of the equidimensional aggregates equal one cm this height is 1.633 cm.
- Minimum and maximum matric suctions are 1.017 and 2180 mbar, respectively, when the diameter of the equidimensional aggregates is one cm.
- Though the program may be used to investigate the relative importance of e.g. soil moisture characteristics or other aggregate diameters on anaerobiosis, such action would demand some recalculations of function tables.

13. COMPUTER

The model may be run on any computer that has a CSMP-III compiler available. These will be in general IBM machines (series 360 and 370) but for some other brands the same package is available (for instance DEC-10).

14. PROGRAM LANGUAGE

CSMP-III. However, the program may be rewritten in FORTRAN-4.

15. RUNNING TIME/COST

Costs were not registrated, but a run took about 120 sec CPU-time.

16. USERS

The model so far is only used by the developer.

17. DEVELOPER AND PRINCIPAL CONTACT

Department of Theoretical Production Ecology
Bornsesteeg 65, 6708 PD Wageningen, the Netherlands

18. REFERENCES

Currie, J.A., 1961. Gaseous diffusion in the aeration of aggregated soils. Soil Science 92: 40-45.

Green, R.E., & J.C. Corey, 1971. Calculation of hydraulic conductivity: A further evaluation of some predictive methods. Soil Science Society of America Proceedings 35: 3-7.

Keulen, H. van, & G.G.E.M. van Beek, 1971. Water movement in layered soils. Netherlands Journal of Agricultural Science 19: 138-153.

Leffelaar, P.A., 1977. A theoretical approach to calculate the anaerobic volume fraction in aerated soil in view of denitrification. A computer simulation study. Report no. 9, Department of Theoretical Production Ecology, Agricultural University, Wageningen, The Netherlands.

Leffelaar, P.A., 1979. Simulation of partial anaerobiosis in a model soil in respect to denitrification. Soil Science 128: 110-120.

Millington, R.J., & R.C. Shearer, 1971. Diffusion in aggregated porous media. Soil Science 111: 372-378.

4.15 A model of denitrification in aggregated soils

K.A. Smith

1. NAME OF MODEL

No name has been given to this model[1] hitherto, but the name AMAZON (A Model of the extent of Anaerobic Zones in soil and the effects on Nitrogen loss by denitrification) has now been coined and will be used in future developments of the model.

2. SYSTEM MODELLED

An assembly of soil aggregates with log-normal distribution of aggregate sizes such as occurs in field soils (Gardner, 1956; Allmaras et al., 1965; Smith, 1977, 1980). Relatively better drainage and aeration occurs in the inter-aggregate pores than within the aggregates (Avery, 1964; Thomasson and Robson, 1967), and if respiratory demand for oxygen exceeds supply, anaerobic zones develop at the centres of the larger aggregates. Denitrification occurs within these zones, resulting in the evolution of nitrous oxide and nitrogen (Smith and Dowdell, 1974; Dowdell and Smith, 1974).

3. OBJECTIVE

To calculate the extent of anaerobiosis from given values of gaseous diffusion coefficients within and between aggregates, aggregate size distribution parameters, temperature and respiration rate, and then to calculate the rates of denitrification occurring in anaerobic zones.

4. TIME SCALE

The model in its present form is applicable only to equilibrium conditions.

5. DIAGRAMS

The pathways of gas diffusion in an assembly of soil aggregates are shown diagrammatically in Fig. 1. There is a critical aggregate size for the development of an anaerobic zone; the fraction of the aggregate volume which is anaerobic rises rapidly with further increase in size (Fig. 2).

---

[1] The model presented here is an abbreviated version of the one published in Journal of Soil Science (Smith, 1980), and is reproduced with the permission of the publishers, Oxford University Press, Oxford.

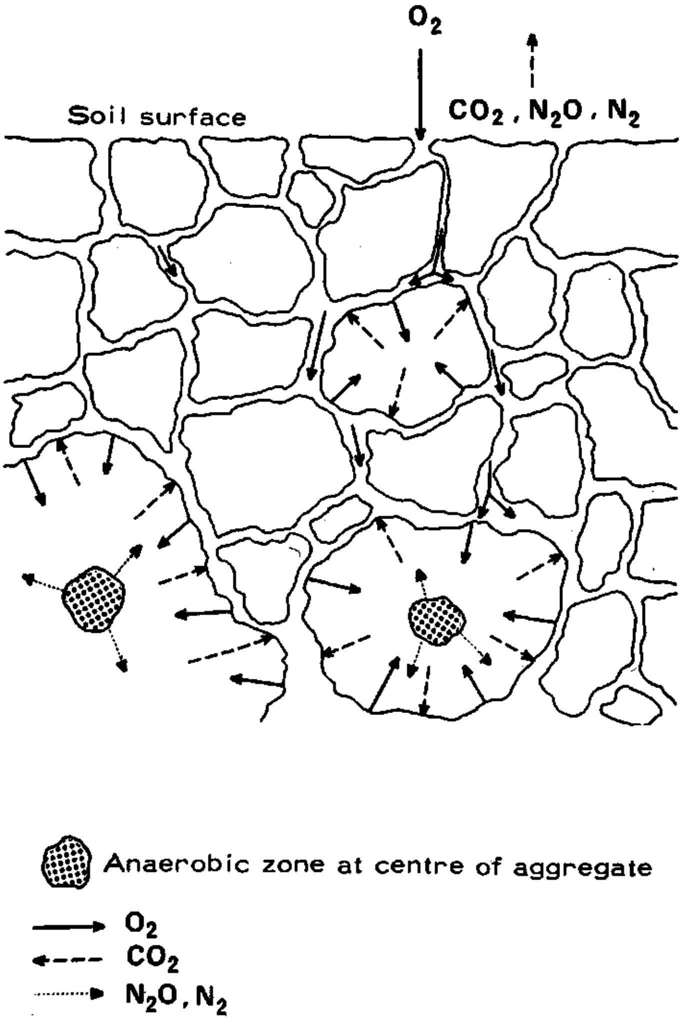


Fig. 1. Diagrammatic representation of gas diffusion pathways in aggregated soil, leading to the formation of anaerobic zones within the larger aggregates.

6. LEVELS

See 7.

7. GOVERNING EQUATIONS

a. *Diffusion within soil aggregates*

The equation for diffusion of oxygen into a spherical aggregate is:

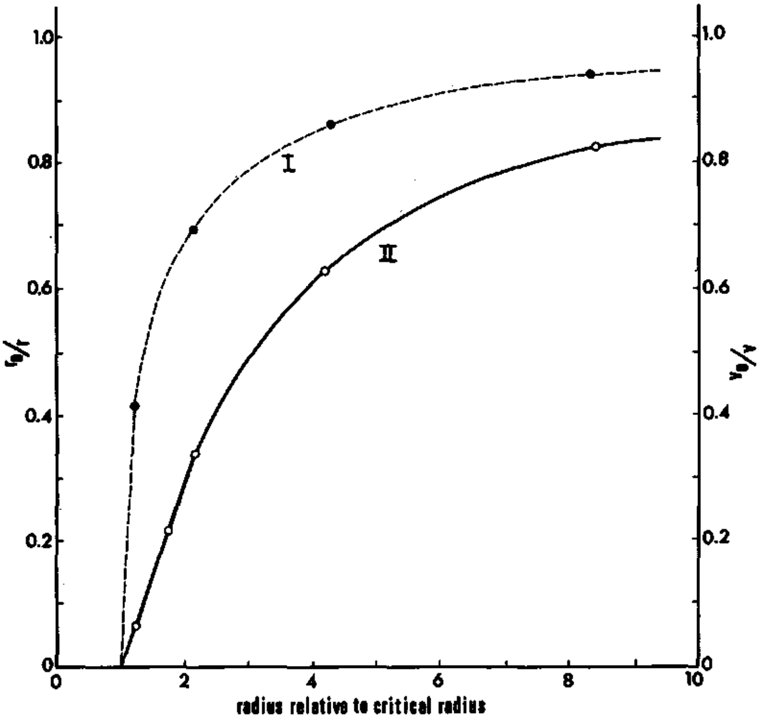


Fig. 2. The relationship between aggregate radius and the fraction of the aggregate volume which is anaerobic.
I: r_o/r; II: $(r_o/r)^3 = v_o/v$.
(From Smith, 1977, reproduced by permission of the Williams and Wilkins Co.)

$$\frac{dc}{dt} = \frac{1}{r^2}\frac{d}{dr}\left[D_a r^2 \frac{dc}{dr}\right] - Q \tag{1}$$

where

r = the radius of the aggregate
c = the concentration of oxygen in the pore space
D_a = the diffusion coefficient within the aggregate
Q = the rate of uptake of oxygen per unit volume of aggregate.

At equilibrium $dc/dt = 0$, thus

$$\frac{d}{dr}\left[r^2 \frac{dc}{dr}\right] = \frac{Qr^2}{D_a} \tag{2}$$

If the anaerobic zone at the centre of the aggregate has a radius r_o, $c = 0$ and

$dc/dr = 0$ when $r = r_o$. Integrating (2) and applying these boundary conditions gives

$$r^2 - 3r_o^{\,2} + \frac{2r_o^{\,3}}{r} = \frac{6D_aC}{Q} \tag{3}$$

where C is the concentration of oxygen in the pore space at the surface of the aggregate (cf Currie, 1961; Greenwood and Berry, 1962).

When the aggregate is just wholly aerobic, $r_o = 0$, and

$$r = r_c = \left[\frac{6D_aC}{Q}\right]^{\frac{1}{2}}$$

r_c is therefore the radius of the largest aggregate which can exist in a wholly aerobic state, for given values of D_a, C and Q. For water-saturated aggregates, C is replaced by C.S, where S is the solubility of oxygen. The fraction of an aggregate of radius r that is anaerobic is $(r_o/r)^3$, where r_o/r is given by

$$r_o/r = -2 \cos \alpha/\cos (\alpha/3) \tag{4}$$

and where $\alpha = -\sin^{-1} (r_o/r)$.

For a log-normal distribution, the fractional volume consisting of aggregates of radius between $r - \frac{\delta r}{2}$ and $r + \frac{\delta r}{2}$ is given by

$$\delta v_r = \frac{1}{\delta r \sqrt{2\pi}} \exp \left[- \frac{(\log r - \log \mu)^2}{2\sigma^2}\right] \delta r \tag{5}$$

where

μ = the mean radius

σ = the (log) standard deviation.

The fractional volume of soil consisting of aggregates of radius r that is anaerobic is given by the product of (4) and (5), i.e. $(r_o/r)^3\ \delta v_r$. The fraction ϕ of the total aggregate volume which is anaerobic is obtained by substituting for δv_r and integrating:

$$\phi = \frac{1}{\sigma\sqrt{2\pi}} \int_{r_c}^{\infty} \frac{r_o^{\,3}}{r^4} \exp \left[- \frac{(\log r - \log \mu)^2}{2\sigma^2}\right] dr \tag{6}$$

where, as above, $r_c = \left[\frac{6D_aC}{Q}\right]^{\frac{1}{2}}$ (Smith, 1980).

b. *Diffusion of oxygen down soil profile*

The relationship between oxygen concentration C and depth x in a uniformly respiring soil is given by

$$\frac{d^2C}{dx^2} - \frac{Q}{D}(1-\varepsilon) = 0 \tag{7}$$

(after Radford and Greenwood, 1970).

In a profile containing anaerobic zones in which no respiration takes place, this becomes

$$\frac{d^2C}{dx^2} - \frac{Q}{D}(1-\varepsilon)(1-\phi) = 0 \tag{8}$$

where

ε = the inter-aggregate porosity

D = the mean diffusion coefficient along the vertical axis through a representative cross-section of soil.

By integration, the relationship between C and x can be determined.

c. *Diffusion of N_2O and N_2*

Let the rate of formation of N_2O/unit anaerobic volume = P. If the rate of formation of N_2 from N_2O = P', then rate of release of N_2O = $P - P'$.

At equilibrium, rate of entry of N_2O into gaseous phase = rate of loss, and the relationship between concentration and depth is given by

$$\frac{d^2C'}{dx^2} + \frac{(P-P')}{D'}(1-\varepsilon)\phi = 0 \tag{9}$$

where

ϕ = the anaerobic volume

ε = the inter-aggregate porosity

C' = the concentration of nitrous oxide

D' = the mean diffusion coefficient for N_2O along the vertical axis through a representative cross-section of soil.

The corresponding diffusion equation for N_2 is

$$\frac{d^2C''}{dx^2} + \frac{P'}{D''}(1-\varepsilon)\phi = 0 \tag{10}$$

where

C'' = the concentration of N_2
D'' = the mean diffusion coefficient for N_2.

d. *Diffusion of nitrate into anaerobic zones*

Assuming that the concentration of nitrate in the anaerobic zone is zero, the quantity F diffusing into the zone per unit time is given by the standard equation for diffusion through a spherical shell (Crank, 1975, p. 89):

$$F = 4\pi D_N \frac{r\,r_o}{r - r_o} C_N \tag{11}$$

where

D_N = the diffusion coefficient for nitrate in solution
r_o = the radius of the anaerobic zone
C_N = the concentration of nitrate near the outer (aerobic) surface of the aggregate.

Assuming that the rate of denitrification is equal to the rate of arrival of nitrate in the anaerobic zone, this rate, per unit volume of aggregate of radius r,

$$= 4\pi D_N C_N \left[\frac{r\,r_o}{r - r_o} \Big/ \frac{4\pi r^3}{3} \right] = 3 D_N C_N \frac{r_o}{r^2(r - r_o)} \tag{12}$$

Thus the total rate for all aggregates of radius r is given by the product of (12) and δv_r (from Equation (3))

$$= 3 D_N C_N \frac{r_o}{r^2(r - r_o)} \; \frac{1}{\delta r\sqrt{2\pi}} \; \exp \left[- \frac{(\log r - \log \mu)^2}{2\sigma^2} \right]$$

and the total rate N for all aggregates is given by

$$N = \frac{3 D_N C_N}{\sigma\sqrt{2\pi}} \int_{r_c}^{\infty} \frac{r_o}{r^3(r - r_o)} \; \exp \left[- \frac{(\log r - \log \mu)^2}{2\sigma^2} \right] dr \tag{13}$$

Thus an estimate of the total denitrification rate may be obtained which can be compared with that derived from the gaseous diffusion equations.

8. INPUT PARAMETERS

C, C', C''	concentrations of oxygen, nitrous oxide and nitrogen, respectively
D_a	diffusion coefficient for O_2 within soil aggregates ($cm^2.s^{-1}$)
Q	rate of oxygen uptake per unit volume of aggregate ($cm^3\ O_2\ s^{-1}.cm^{-3}$)
D, D', D''	diffusion coefficients for O_2, N_2O, N_2, respectively, between aggregates (i.e. through the soil profile) ($cm^2.s^{-1}$)
S	solubility of oxygen in water ($cm^3.\ cm^{-3}$)
T	temperature (°C)
μ	mean aggregate radius (cm)
σ	(log) standard deviation of aggregate size distribution
ε	inter-aggregate porosity ($cm^3.cm^{-3}$)
C	concentration of nitrate ($g.cm^{-3}$)
D_N	diffusion coefficient for nitrate in solution ($cm^2.s^{-1}$)

9. OUTPUT VARIABLES

ϕ	the fraction of the total volume which is anaerobic
P	the rate of formation of N_2O
P'	the rate of formation of N_2
N	the total rate of denitrification as indicated by the disapperance of nitrate

10. OBSERVATIONS

Theoretical model only - not yet tested experimentally.

12. LIMITS AND LIMITATIONS

D_a is within the range 10^{-6} to 10^{-2} $cm^2.s^{-1}$.

D is within the range 7.6×10^{-6} s^{-1} to 7.6×10^{-2} $cm^2.s^{-1}$.

C is within the range 0 to 0.21 $cm^3.cm^{-3}$.

μ, σ, ε, D_a, D, Q and C_N are assumed to be constant with depth.

It is further assumed that the actively respiring soil is of sufficient depth to ensure that the inter-aggregate oxygen concentration reaches zero.

The selection of values for the parameters above is discussed in Smith (1980).

13. COMPUTER

SYSTIME 5000 (based on PDP 11-34).

14. PROGRAM LANGUAGE

BASIC

15. RUNNING TIME

Approx. 3 minutes (to give values of ϕ for 10 values of C). Should be similar for other calculations - not yet run.

16. USERS

Developer only, but usable by anyone.

17. DEVELOPER

K.A. Smith, Edinburgh School of Agriculture, West Mains Road, Edinburgh EH9 3jG, U.K.

REFERENCES

Allmaras, R.R., R.E. Burwell, W.B. Voorhees, and W.E. Larson, 1965. Aggregate size distribution in the row zone of tillage experiments. Soil Science Society of America Proceedings 29: 645-650.

Avery, B.W., 1964. The soils and land use of the district around Aylesbury and Hemel Hempstead. (Sheet 238.) Memoirs of Soil Survey of England and Wales, H.M.S.O., London, 216 p.

Crank, J., 1975. The mathematics of diffusion, 2nd ed., Oxford University Press, London, 414 p.

Currie, J.A., 1961. Gaseous diffusion in the aeration of aggregated soils. Soil Science 92: 40-45.

Dowdell, R.J., and K.A. Smith, 1974. Field studies of the soil atmosphere. II. Occurrence of nitrous oxide. Journal of Soil Science 25: 231-238.

Gardner, W.R., 1956. Representation of soil aggregate-size distribution by a logarithmic-normal distribution. Soil Science Society of America Proceedings 20: 151-153.

Greenwood, D.J., and G. Berry, 1962. Aerobic respiration in soil crumbs. Nature 195: 161-163.

Radford, P.J., and D.J. Greenwood, 1970. The simulation of gaseous diffusion in soils. Journal of Soil Science 21: 304-313.

Smith, K.A., 1977. Soil aeration. Soil Science 123: 284-291.

Smith, K.A., 1980. A model of the extent of anaerobic zones in aggregated soils, and its potential application to estimates of denitrification. Journal of Soil Science 31: 263-277.

Smith, K.A., and R.J. Dowdell, 1974. Field studies of the soil atmosphere. I. Relationship between ethylene, oxygen, soil moisture content and temperature. Journal of Soil Science 25: 219-230.

Thomasson, A.J., and J.D. Robson, 1967. The moisture regimes of soils developed on Keuper Marl. Journal of Soil Science 18: 329-340.

5. Appendixes

5.1 Some mathematical tools and programming procedures for soil simulations

V. Amdursky, I. Tzur and A. Ziv

1. INTRODUCTION

Our aim is to describe certain mathematical tools which have been especially developed in order to achieve short computer runtime for a soil simulation.

The model used is the one described in J. Hagin and A. Amberger (1974), and in G. Kruh and E. Segall (1980), which was originally programmed in CSMP.
We shall limit ourselves to the brief description of some mathematical tools which enabled a reduction of runtime by an order of magnitude, and in addition, enabled the obtaining of results in situations which the former computer program could not handle, independently of runtime. The purpose of this paper is mainly to represent 'recepies', and not to provide a complete mathematical background and justification.

We refer, however, to V. Amdursky (1980) where the underlying mathematical theory is described, and which may be applied in case certain problematic equations of a different character have either to replace or be added to the present ones.
Due to space limitations, only the main ideas will be presented, leaving aside technical details of secondary importance.

2. SOURCES OF DIFFICULTY AND GENERAL DESCRIPTION OF THE PROGRAM

Although some of the equations appearing in the model are basically partial differential equations, they have been discretized (in space) already in the previous CSMP program, and we decided to accept this spatial discretization without any modification, so that the entire model is now formulated as a system of ordinary differential equations, with time as the independent variable. In attempting to solve these equations numerically, the following difficulties arise:
1. The presence of 'stiff' equations, in the ordinary sense.
2. The presence of highly oscillatory terms, on the right-hand-sides of some equations, this being combined with 'stiffness'.
3. The necessity to handle quite many 'transition points', i.e., points on the time axis in which a sudden discontinuity is introduced, and moreover, some of the expressions appearing on the right-hand-sides are replaced by (more or less) different ones, thus

introducing sharp 'boundary layers'. In our simulation, such 'transition points' are due to the following:

a. The beginning or the termination of rain or irrigation.

b. The beginning or the termination of a state of flooding.

The latter situation is especially critical, since this implies a sudden drop in oxygen concentration, and usually, a denitrification process resulting from it.

One point should be made clear at the very beginning: Even when treating the differential equations which exhibit ordinary stiffness, most of the difficulties are not due to stability but rather to accuracy problems arising from the slow accumulation of errors over a long period of time (100 days as a typical period). It is for this reason that ordinary methods originally devised for stiff equations can be used only for some equations, but most of the difficulties will still remain. Moreover, even for these equations the usual methods devised for stiff equations fail to handle the 'boundary-layers'.

The main features of the present program are the following:

1. The simultaneous usage of four different, specially tailored methods of integration.
2. The usage of a certain 'block' in the program, called 'sensors', whose task is to predict-ahead the points in time where sudden (sharp) discontinuities or boundary-layers are to occur, and to make all the preparations needed for tackling this situation.

3. SOME INTEGRATION METHODS

(A) We start by describing the method of integration which we apply both for the concentration of oxygen and for the water content in the upper (1 & 2 in our case) layers of soil.

Assume that we have to solve a system of equations of the following type:

$$\dot{Y} = A(t)\cdot Y + B(t)$$

$$Y(t_o) = Y_o$$

over a relatively 'small' time interval $(t_o, t_o + \Delta t)$ which, in turn, may be 'large' compared to $1/\lambda$ (λ being any eigenvalue of A). However, we seek a method which will have the following properties:

1. The method should be applicable also in the 'boundary-layer' stage.
2. The method should be applicable independently of the size of (λ) - that is - both for small, medium or large values of λ. We assume, however, that the values of λ are always non-positive, real numbers.

Actually, A and B are not given as explicit functions of time; on the contrary, they depend both on time in an explicit way, and implicitly on it via some explicit definition in terms of the entire vector of unknown variables of the simulation, including Y itself and many other unknowns. We assume, however, on physical grounds, that A(t) and B(t) are relatively 'moderately varying'. We shall come to this point later on. Meanwhile, let us assume A, B to be given explicitly as functions of time. Moreover, we assume $A(t_o)$ to have a diagonal Jordan form:

$$A(t_o) = V\Lambda V^{-1}$$

We now define the following

$$\overset{*}{A} \equiv {}_{\Delta}A(t_o)$$

$$\overset{*}{B} \equiv {}_{\Delta}B(t_o) - V[(e^{\Lambda\Delta t} - I)^{-1}\,\Delta t - \Lambda^{-1}]V^{-1}\,[B'(t_o) + A'(t_o)Y_o]$$

Let Z = Z(t) denote the analytical solution of the following linear equation with constant coefficients:

$$\dot{Z} = \overset{*}{A}Z + \overset{*}{B}$$

$$Z(t_o) = Y_o$$

We study the difference Y(t) - Z(t). Assuming $V^{-1}(t_o)$, $V(t_o)$, $B(t_o)$, B'(t), A'(t), B"(t), A"(t) to be 0(1) over $(t_o,\ t_o + \Delta t)$ (which we shall call 'nice behaviour'), and assuming the elements of Λ to be non positive, one can prove the following (somewhat roughly stated) assertion:

a. Beyond the boundary layer, we have $Y-Z = 0(\Delta t^3)$ throughout $(t_o,\ t_o + \Delta t)$; this also holds within the boundary layer in case $\Lambda = 0(1)$.

b. Within the boundary layer we have at least $Y-Z = 0(\Delta t^2)$, and even much better in case the elements of Λ are all large.

It is because of these error estimates that one may use the analytical solution Z(t), within $(t_o,\ t_o + \Delta t)$, as a good approximation to Y(t), which meets our requirements (1), (2) mentioned before, and this is actually what we do in the program.
In order to obtain $B'(t_o)$, $A'(t_o)$, we use, due to their 'nice behaviour', a backward interpolation & differentiation 1-order scheme, which is not very critical and this can be justified since A"(t), B"(t) = 0(1). This is why the actual dependence of A and B on the entire vector of unknowns does not bother us. It should be mentioned, however, that when this 'nice behaviour' of A, B in $(t_o,\ t_o + \Delta t)$ does not hold, one needs more clever devices, but we shall not enter this matter here.

(B) Another difficult problem arises with the computation of soil temperatures over long periods of time. Having introduced the spatial discretization, one encounters the following type of a scalar differential equation for the temperature of the upper layer of soil:

$$\frac{dZ}{dt} = \lambda(t)Z + B(t) + A(t)T(t)$$

where λ may obtain relatively 'large' negative values; $B(t)$, $A(t)$, $\lambda'(t)$ have nice behaviour, but $T(t)$ is highly oscillatory on a long-period scale. This oscillatory nature stems from the day-to-night changes in atmospherical conditions.
The numerical solution, even when using methods devised for stiff differential equations, becomes rather problematic due to the accumulation of errors. One needs a rather accurate method, on a local scale, in order to prevent this accumulation on a global scale.

Again, as in (A), the coefficients λ, A, B actually depend on other variables appearing in the system, but meanwhile we disregard this fact.

We proceed as follows: $T(t)$ is a priori given in the simulation via a discrete table of (measured) specified temperatures. For a continuous representation, we use a chain of splines of the fifth degree, each spline serving over a period of 12 hours. This provides a very good, detailed and smooth description of $T(t)$ over the entire period. Assuming this representation to be exact, the analytical solution for $Z(t)$ is given by

$$Z(t_o + \Delta t) = e^{\int_{t_o}^{t_o+\Delta t} \lambda(\tau)d\tau} Z(t_o) + \int_{t_o}^{t_o+\Delta t} e^{\int_{\tau}^{t_o+\Delta t} \lambda(\xi)d\xi} [B(\tau) + A(\tau)T(\tau)]\, d\tau$$

write: $\lambda_o \equiv {}_{\Delta}\lambda(t_o)$.
Then $Z(t_o + \Delta t)$ may be written as follows:

$$Z(t_o + \Delta t) = Z(t_o)e^{\lambda_o \Delta t}\, e^{\int_{t_o}^{t_o+\Delta t} (\lambda(\tau)-\lambda_o)d\tau} + \int_{t_o}^{t_o+\Delta t} e^{\lambda_o(t_o+\Delta t-\tau)}$$

$$\cdot\, e^{\int_{\tau}^{t_o+\Delta t} (\lambda(\xi)-\lambda_o)d\xi} [B(\tau) + A(\tau)T(\tau)]\, d\tau$$

Due to the nice behaviour of $\lambda'(t)$, $B(t)$, $A(t)$, we may very well approximate $(\lambda(\tau)-\lambda_o)$;

$$e^{\int_{\tau}^{t_o+\Delta t}(\lambda(\xi)-\lambda_o)d\xi} B(\tau); \quad e^{\int_{\tau}^{t_o+\Delta t}(\lambda(\xi)-\lambda_o)d\xi} A(\tau)$$

over $(t_o, t_o + \Delta t)$ by polynomials obtained from backward information stored in computer's memory, and these are denoted by $\overline{M}(\tau)$, $\overline{A}(\tau)$, $\overline{B}(\tau)$ respectively.

Let $P(\tau)$ denote the (picewise) polynomial $\overline{B}(\tau) + \overline{A}(\tau) \cdot T(\tau)$. We are now faced with the problem of computing

$$\int_{t_o}^{t_o+\Delta t} e^{\lambda_o(t_o+\Delta t-\tau)} P(\tau)d\tau.$$

Let $P(\tau)$ be rearranged in powers of $(\tau-(t_o+\Delta t))$ as

$$P(\tau) \equiv \sum_{s=0}^{r} a_s(\tau-(t_o+\Delta t))^s$$

Successive integration by parts yields then the following exact formula:

$$\int_{t_o}^{t_o+\Delta t} e^{\lambda_o(t_o+\Delta t-\tau)} P(\tau)d\tau + \sum_{j=0}^{r} (j!/\lambda_o^{j+1}) \left[\sum_{s=j}^{r} a_s \binom{s}{j} (e^{\lambda_o \Delta t}(-\Delta t)^{s-j} - a_j \right]$$

so that

$$Z(t_o+\Delta t) \cong Z(t_o)e^{\lambda_o \Delta t} e^{\int_{t_o}^{t_o+\Delta t} \overline{M}(\tau)d\tau} + \sum_{j=0}^{r} (j!/\lambda_o^{j+1}) \left[\sum_{s=j}^{r} a_s \binom{s}{j} \cdot (e^{\lambda_o \Delta t}(-\Delta t)^{s-j} - a_j \right]$$

A careful error analysis shows that if $\overline{A}$, $\overline{B}$, $\overline{M}$ are approximations of order $(O(\Delta t^{\ell+1})$ over $(t_o, t_o + \Delta t)$, then the error in Z is $O(\Delta t^{\ell+2})$, (and in case of large values of λ it is even better).

Certain precautions must be taken when changing from any spline to the next one, but we shall not discuss this matter here.

(C) The third integration method which we use handles a system of ordinary differential equations which arises from spatial discretization of diffusion equations:

$$\frac{dY}{dt} = A(t)Y + B(t)$$

In this case, however, A(t) is a tridiagonal matrix. Again A(t), B(t) depend actually also on the unknown variables of the simulation. We use a modified Crank-Nicholson scheme ('implicit trapezoidal') as follows: the values of $Y(t+\Delta t)$ are determined from:

$$Y(t+\Delta t) - Y(t) = \{[A(t)Y(t) + B(t)] + [A(t+\Delta t)Y(t+\Delta t) + B(t+\Delta t)]\} (\Delta t/2).$$

The values of $B(t+\Delta t)$, $A(t+\Delta t)$ are obtained from first-order extrapolation of backward information, and the values of $Y(t+\Delta t)$ are determined from the well known elimination method existing for tridiagonal linear algebraic equations, which requires a computational effort which is linear in the dimension of Y. This method is used both for the water content and for the concentration of oxygen in the layers of soil other than the 1 and 2, and for the temperatures in all the layers exept the first one. It is stable and accurate to the second order in Δt. Sharp boundary layers show up only in the upper layers, and these are handled by other integration methods.

(D) The fourth integration which we use is a variable step Adams Bashforth method.

3. SOME PROGRAMMING ASPECTS

The program is now written in Fortran. Due to the integration methods used, each time step requires only a single computation of the right-hand-sides, which is done via a separate subroutine. Each integration method appears as a separate subroutine, and the same is true also for the 'sensors'. Backward information is stored according to the instructions of a special 'block' in the program.

REFERENCES

Hagin, J., and A. Amberger, 1974. Contribution of fertilizers and manures to the N- and P-load of waters - a computer simulation, Final Report submitted to the Deutsche Forschungs Gemeinschaft.

Kruh, G., and E. Segall, 1980. Nitrogen dynamics in soil, this publication.

Amdursky, V., 1980. A tool for differential equations with a small parameter, IBM Israel Scientific Center Technical Report 081.

5.2 Survey of workshop participants

ORGANIZATION

Dr. M.J. Frissel
Dr. J.A. van Veen
Mr. P. van Nierop

WORKSHOP CHAIRMAN

Dr. J.H. Rayner

PARTICIPATING WORKSHOP MEMBERS

Dr. T.M. Addiscott, Rothamsted Experimental Station, Harpenden, Herts. AL5 2JQ, United Kingdom.
Dr. V. Amdursky, IBM Israel Scientific Center, Haifa 32000, Israel.
Dr. E. Bosatta, Swedish Coniferous Forest Project, Box 7042, S-75007 Uppsala, Sweden.
Dr. H. Breteler, Foundation ITAL, P.O. Box 48, 6700 AA Wageningen, The Netherlands.
Dr. J.M. Davidson, University of Florida, 2169 McCarty Hall, Gainesville, Florida 32611, U.S.A.
Ir. P. de Willingen, Institute for Soil Fertility, Oosterweg 92, 9750 RA Haren, The Netherlands.
Dr. M.J. Frissel, Foundation ITAL, P.O. Box 48, 6700 AA Wageningen, The Netherlands.
Dr. D.J. Greenwood, National Vegetable Research Station, Wellesbourne, Warwick CV35 9EF, United Kingdom.
Dr. K. Harmsen, ICARDA, P.O. Box 5466, Aleppo, Syria.
Dr. I.K. Iskandar, Dept. of the Army, U.S. Army Cold Regions Research and Engineering Lab., P.O. Box 282, Hanover, New Hampshire 03755, U.S.A.
Mr. N.G. Juma, Dept. of Soil Science, University of Saskatchewan, Saskatoon, Saskatchewan, S7N 0W0, Canada.
Ir. G.J. Kolenbrander, Institute for Soil Fertility, Oosterweg 92, 9750 RH Haren, The Netherlands.
Dr. G. Kruh, Soils and Fertilizer Div., Technion Israel Inst. of Technology, Haifa 32000, Israel.

Ir. P.A. Leffelaar, Dept. of Theoretical Crop Production, State Agricultural University, Bornsesteeg 65, 6708 PD Wageningen, The Netherlands.

Dr. W.J. Parton, Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Mr. I. Petterson, Dept. of Ecology and Environmental Management, Swedish University of Agricultural Sciences, S-75007 Uppsala, Sweden.

Dr. P.S.C. Rao, University of Florida, 2169 McCarty Hall, Gainesville, Florida 32611, U.S.A.

Dr. J.H. Rayner, Rothamsted Experimental Station, Harpenden, Herts. AL5 2JQ, United Kingdom.

Dr. J.O. Reuss, Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Dr. J.S. Russell, CSIRO, Division of Tropical Crops and Pastures, Cunningham Laboratory, Queensland 4067, Australia.

Dr. D. Sauerbeck, Institut für Biochemie des Bodens, Bundesforschungsanstalt für Landwirtschaft, Bundesallee 50, Braunschweig - Volkenrode, B.R.D.

Dr. I. Shvytov, Resource and Environmental Area, International Institute for Applied Systems Analysis, A-2361 Laxenburg, Austria.

Dr. K.A. Smith, Edinburgh School of Agriculture, West Mains Road, Edinburgh, United Kingdom.

Dr. K.K. Tanji, Land, Air and Water Resources, 113 Veihmeyer Hall, University of California, Davis, California 95616, U.S.A.

Dr. F. van Dorp, Foundation ITAL, P.O. Box 48, 6700 AA Wageningen, The Netherlands.

Ir. H.G. van der Meer, Centre for Agro-biological Research, P.O. Box 14, 6700 AA Wageningen, The Netherlands.

Dr. H. van Keulen, Centre for Agro-biological Research, P.O. Box 14, 6700 AA Wageningen, The Netherlands.

Dr. J.A. van Veen, Foundation ITAL, P.O. Box 48, 6700 AA Wageningen, The Netherlands.

Dr. R.J. Wagenet, Soil Science and Biometeorology, Utah State University, Logan, Utah 84322, U.S.A.

NON-PARTICIPATING (CO-)AUTHORS

Dr. F.J. Adamsen, Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Dr. L. Bringmark, Dept. of Plant Ecology, University of Lund, S-22362 Lund, Sweden.

Dr. S.K. Gupta, Dept. of Land, Air and Resources, University of California, Davis, California 95616, U.S.A.

Dr. W.D. Gould, Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Dr. H.W. Hunt, Dept. of Biology, West Virginia University, Morgantown, West Virginia, U.S.A.

Dr. R.E. Jessup, Soil Science Dept., University of Florida, Gainesville, Florida 32611, U.S.A.

Dr. W.B. McGill, Dept. of Soil Science, University of Alberta, Edmonton, Alberta, Canada.

Dr. M. Mehran, Dept. of Land, Air and Water Resources, University of California, Davis, California 95616, U.S.A.

Dr. E.A. Paul, Dept. of Soil Science, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 0W0.

Dr. K.H. Paustian, Dept. Ecology and Environmental Research, Swedish University of Agricultural Sciences, Uppsala, Sweden.

Dr. E. Segal, Computer Center, Technion, Haifa, Israel.

Dr. Noam Seligman, Agricultural Research Organization, Volcani Center, Bet Dagan, Israel.

Dr. H.M. Selim, Agronomy Dept. Louisiana State University, Baton Rouge, Louisiana, U.S.A.

Dr. H. Staaf, Dept. of Plant Ecology, University of Lund, S-22362 Lund, Sweden.

Dr. S. Torbit, Natural Resource Ecology Laboratory, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Mr. I. Tzur, M. Sc. IBM Israel Scientific Center, Haifa 32000, Israel.

Dr. O.F. Vasiliev, Resource and Environmental Area, International Institute for Applied System Analysis, A 2361 Laxenburg, Austria.

Dr. R.W. Woodmansee, Dept. of Range Science, Colorado State University, Fort Collins, Colorado 80523, U.S.A.

Dr. A. Zif, IBM Israel Scientific Center, Haifa 32000, Israel.