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A HYDRO-QUALITY MODEL TO PREDICT THE EFFECTS OF BIOLOGICAL TRANSFORMATIONS ON THE CHEMICAL QUALITY OF RETURN FLOW

by

V. A. Narasimhan

A dissertation submitted in partial fulfillment
of the requirements for the degree

of

DOCTOR OF PHILOSOPHY

in

Engineering

Approved:

Major Professor	Committee Member
Committee Member	Committee Member
Committee Member	Dean of Graduate Studies

UTAH STATE UNIVERSITY
Logan, Utah

1975

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V. A. Narasimhan

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by

V. A. Narasimhan, Doctor of Philosophy

Utah State University, 1975

Major Professor: Dr. J. Paul Riley
Department: Civil and Environmental Engineering

A computerized mathematical model has been developed to simulate the system hydrology and water-salinity (as indicated by seven major ions constituting the salt) of a river basin, in which irrigation is the major beneficial water user. The overall system simulation model consists of three submodels: (1) a general hydrologic submodel programmed on a hybrid computer; (2) a chemical submodel to predict the quality of percolated water through the soil profile; and (3) a biological transformation submodel in respect of microbial nitrogen transformations, which is utilized by the chemical submodel. Both the chemical and biological submodels are programmed on a digital computer and are combined with the general hydrologic submodel to form the system simulation model. The overall model operates on monthly time intervals with variable spatial resolution.

The hydrologic portion of the model simulates the various hydrologic processes which are linked together by the continuity-of-mass principle and predicts the monthly runoff from the area. The chemical quality component of the model considers the complex chemistry of soil-water-plant system, including cation exchange on the soil complex, the dissolution or precipitation of lime ($CaCO_3$), and calcium and magnesium sulphates ion pairs in solution.

The biological transformations submodel uses the kinetic approach in simulating the microbial nitrogen transformations within the root zone of a soil profile. The transformation reactions included are: (1) hydrolysis of Urea-nitrogen; (2) immobilization of ammonium-nitrogen; (3) mineralization of organic-nitrogen; and (4) immobilization of nitrate-nitrogen. The chemical composition of return flow is a function of these chemical and biological processes within the soil profile, in addition to blending of undiverted flows, evapotranspiration, and mixing of subsurface return flow with groundwater. Uptake of nitrate by aquatic biomass in the surface runoff of return flow has also been considered. The seven ions considered in the study are calcium, magnesium, sodium, sulphate, chloride, bicarbonate, and nitrate. The total dissolved solids outflow is a summation of these individual ions.

In order to demonstrate its capabilities, the hydro-quality model is applied to a large irrigated area of the Snake River Plains, near Twin Falls, Idaho. The model successfully simulated measured outflows of water and the concentration of seven ions for a 24 month period. The correlation coefficients range from 0.79 to 0.96 for the quantity and quality components of outflow, except for the sulphate ion, the correlation coefficient of which is 0.66. The model is general in nature and with suitable adjustments it can be applied to other areas and also to various kinds of management situations, including land application of waste water and studies involving nitrate pollution of groundwaters.

(201 pages)

CHAPTER I

INTRODUCTION

General

The current rapid growth of demand on the limited water resource places emphasis on the quality of water being used as well as that which returns to the supply to be reused in irrigation or other systems. The water quality dimension, therefore, appears to be the limiting factor in any water reuse. To be able to adequately describe this parameter, it is necessary to identify and evaluate the impact of upstream uses on the quality flow system occurring at downstream points.

Proper evaluation of consequences downstream resulting from upstream changes is difficult because of the complex interrelation and the variable nature of the combined hydrologic and quality flow systems. The quality flow system is itself interrelated with the physical, chemical, and biological subsystems. Any change which brings about a new equilibrium in the quantity flow system brings a corresponding alteration in the quality system. In other words, quantity and quality are the two dimensions of the same problem, depending upon the dynamic characteristics of the hydrologic system and the prevailing water use patterns within the system. Therefore, realistic analysis to this complex problem can lead to increased use and better efficiency of the system.

Among the many water reuse systems, the one of relative importance is an irrigation system. The acreage of land irrigated and the quantity of water consumed are indicative of the magnitude of problems associated with irrigation return flows. The problem of water quality degradation in an irrigation cycle is not limited to the western United States, but is a major problem in many areas of the world. This problem appears in a highly magnified scale, particularly in those portions of the world facing the greatest population pressures requiring high food production within the limited land and water resources.

The detrimental effects of an irrigation system on environmental water quality are a consequence of the many processes involved. Included in these processes are the increased concentration of salts in the return flows on account of consumptive water use by plants and dissolution in soil profile, resulting in both surface and groundwater pollution (mainly from nitrate). The problem of the system is, therefore, one of multidisciplined requiring an analysis of both conservative and nonconservative water quality parameters.

Importance and Timeliness of Research

The problem of water quality degradation has long been recognized, but its impact is felt only in recent years on account of its gradual development requiring research efforts to technically solve this problem. Recently, the Environmental Engineering Research Committee of the Environmental Engineering Division of the ASCE (1973) has emphasized the need for improvements in the techniques for not only the flow characteristics of the injected surface water, but also the distribution and concentration of potential pollutants, namely the nitrate ion, in the percolating waters. Suggestions have also been made in the proceedings of the Ninth Biennial Conference on Groundwater (1973) that in the technique of analysis of the problem, nitrate could popularly be considered as a conservative parameter. A comprehensive technique describing the analyses of physical, chemical, and biological effects on the quality of return flow is, therefore, one of the current topics requiring pooling of knowledge from more than one discipline.

In recent years there is a tremendous increase in the use of mathematical modeling as a problem solving technique under such labels as "systems analysis," "operations research," and "simulation techniques." The problem envisioned herein is, therefore, analyzed with the concepts of systems analysis in developing a comprehensive hydro-quality simulation model to predict the quantity and quality of return flow.

A comprehensive hydro-quality (salinity) model has many advantages, including some of the important ones as mentioned below.

1. It facilitiates inclusion of individual processes which contribute to salinity flow in the system.
2. Sensitivity analysis on these individual processes can result in knowledge of the relative contribution made by each process to the system as a whole.
3. Such knowledge is necessary to make efficient management decisions and to develop control measures which would lead to

reducing the salinity level of return flow.

4. As stated by Orlob (1972), a well conceived comprehensive model can better define a meaningful data program, one that when coupled with a modeling capability, will provide the water resources planner with the needed tools for reliable prediction of future consequences.

Scope of Study

Return flows from an irrigation system can come from surface runoff, or can return to the system through the soil profile. Mathematical models can be developed to represent either of the flow systems or both, depending upon the area of study and the types of problems proposed to be resolved. Also, there is no single factor, physical, chemical, or biological which can be used alone to indicate the quality of a water body. The indicies of water quality depend upon the specific purpose to which the water is used. A basic list of water quality indices that will provide the adequate information required by a large percentage of users is shown by Table 1. Included in this list are some of the most important water quality parameters that would be of concern in a comprehensive hydro-quality model of the return flow system.

Several authors, including Hyatt et al. (1970), Jensen (1971), Thomas et al. (1971), and Hill et al. (1973), have developed mathematical models to predict the quality and quantity of irrigation return flow. None of these models, except that of Thomas et al. (1971), adequately describe a

Table 1. A basic list of water quality indices or parameters.

A. <u>Usual Parameters</u>

- Temperature
- Ammonia
- Dissolved Oxygen
- Nitrate
- BOD
- Phosphate
- Fecal Coliform
- Chlorophyll *a*
- Fecal Streptococci
- TDS
- Turbidity
- PH
- ZooPlankton
- Alkalinity
- Hardness

B. <u>Parameters for special purposes</u>

- Nutrients
- Heavy Metals
- Pesticides
- Herbicides
- Sediment
- Toxics
- Radioactive Nuclides

C. <u>Parameters of concern in return flows</u>

- NO_3^-, Ca^{++}, Mg^{++}, Na^+, Cl^-, $SO_4^=$, HCO_3^-, $PO_4^{\equiv}$, TDS.
- pH
- Pesticides
- Herbicides
- Bacteria

majority of the water quality parameters listed in Table 1. The model developed by Thomas (1971), however, does not consider the distribution of organic and inorganic nitrogen. This study, therefore, considers the chemical quality parameters as effected by biological transformations in respect of microbial nitrogenous species. It has made an effort towards developing a comprehensive hydro-quality (salinity) computer simulation model. The individual ions considered are Ca^{++}, Mg^{++}, Na^{+}, Cl^{-}, HCO_3^{-}, NO_3^{-}, and $SO_4^{=}$.

The research work involved in developing such a model has been the result of a contributing research of the Utah State University to the Western Regional Research Project W-107, "Management of Salt Load in Irrigated Agriculture." The dissertation of this writer involved the final phase of research work in this project.

Objective

The purpose of this study is to develop a general hydroquality computer simulation model in accordance with the following considerations.

1. Develop, list and improve, as required, the fundamental mathematical equations for expressing:
    a. The physical behavior of the dynamic hydrologic processes.
    b. Chemical reactions involving dissolution and precipitation phenomena of different ions in the soil profile.
    c. Effect of biological processes on the chemical reactions, with reference to microbial nitrogen transformations.
2. Utilize a computer to synthesize the various phenomena into a

working model of the hydrologic, chemical, and biological transformation subsystems.

3. Make particular provision to the ability of the model to predict the quantities of the individual ions which comprise the effluent salts.
4. Apply the model so developed to an existing irrigated area to demonstrate the feasibility of this simulation approach for predicting the quality and quantity of return flow.

Procedure

The model utilizes the following submodels:

1. A hydrologic submodel of the irrigated portion of the basin.
2. A chemical submodel to predict the chemical composition of return flow that percolated through the soil profile.
3. A biological transformation submodel to predict the average concentration of NO_3^- ion that will be utilized by the chemical model for the various exchange reactions.

The chemical and biological submodels, including other quality functions, are integrated into the overall hydrologic model. The overall model is, however, verified by comparison of the simulated results with actual field data from an irrigated area near Twin Falls, Idaho (Figure 1).

Discussion

Thomas (1971) has developed a mathematical model of the complex physical and chemical processes occurring in a hydrologic system. The

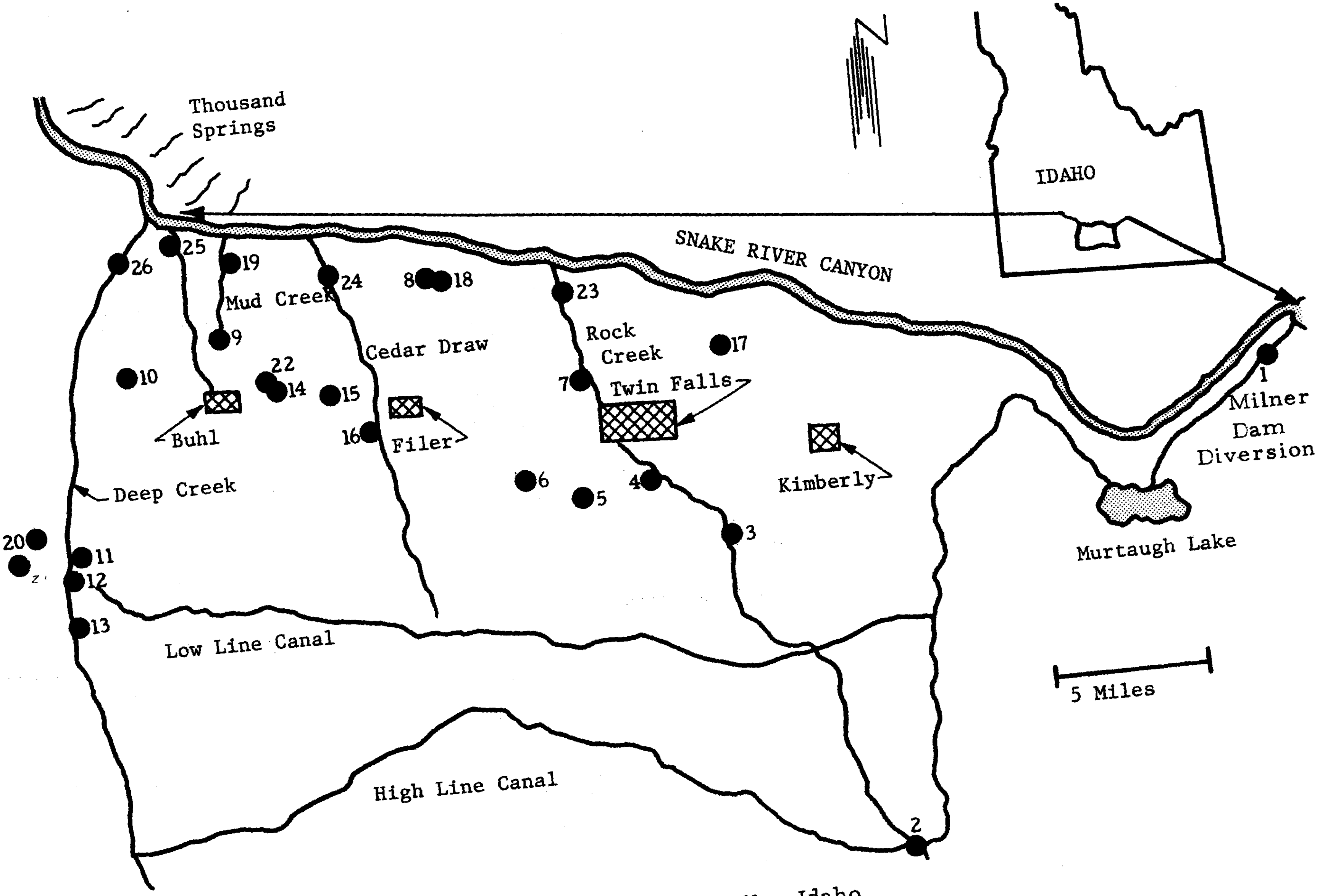


Figure 1. Map of Snake River Basin, Twin Falls, Idaho.

model, however, does not consider the behavior of organic and inorganic nitrogen. Therefore, strictly no mathematical model considering the physical, chemical, and biological processes occurring in a hydrologic system has yet been attempted. This is because of limitations of data, knowledge, and time. The model developed herein is an achievement towards a comprehensive hydroquality model incorporating the physical, chemical, and biological processes in an irrigated land. In order to make the overall modeling procedure as practical as possible, attempts were made to simplify quantitative relationships and reduce the data requirements to an absolute minimum, while still retaining a useful and reasonable representation of the hypothetical system.

CHAPTER II

REVIEW OF LITERATURE

General Considerations

With the advent of legislation requiring the maintenance or improvement of surface water quality in a river regime within the United States, there has been considerable research in recent years on comprehensive water quality modeling, including both the conservative and non-conservative parameters. Several publications, including the one edited by Biswas (1972) and Hydrocomp (1973), describe the capabilities of various water quality models. Hornsby (1973) reviewed the state-of-the-art of prediction modeling for salinity control of a return flow system represented by Figure 2. King and Hanks (1973) developed two types of models, one designed as an irrigation management tool, and the other to provide a detailed understanding of the water and salt flow through the soil.

In terms of a comprehensive water quality model of the return flow system shown by Figure 2, the soil-plant water system needs further analysis to include the transport of essential nutrients, namely the nitrogen. This chapter reviews the techniques evolved by various researchers in respect of microbial nitrogen transformations within the zone of root influence in the soil profile.

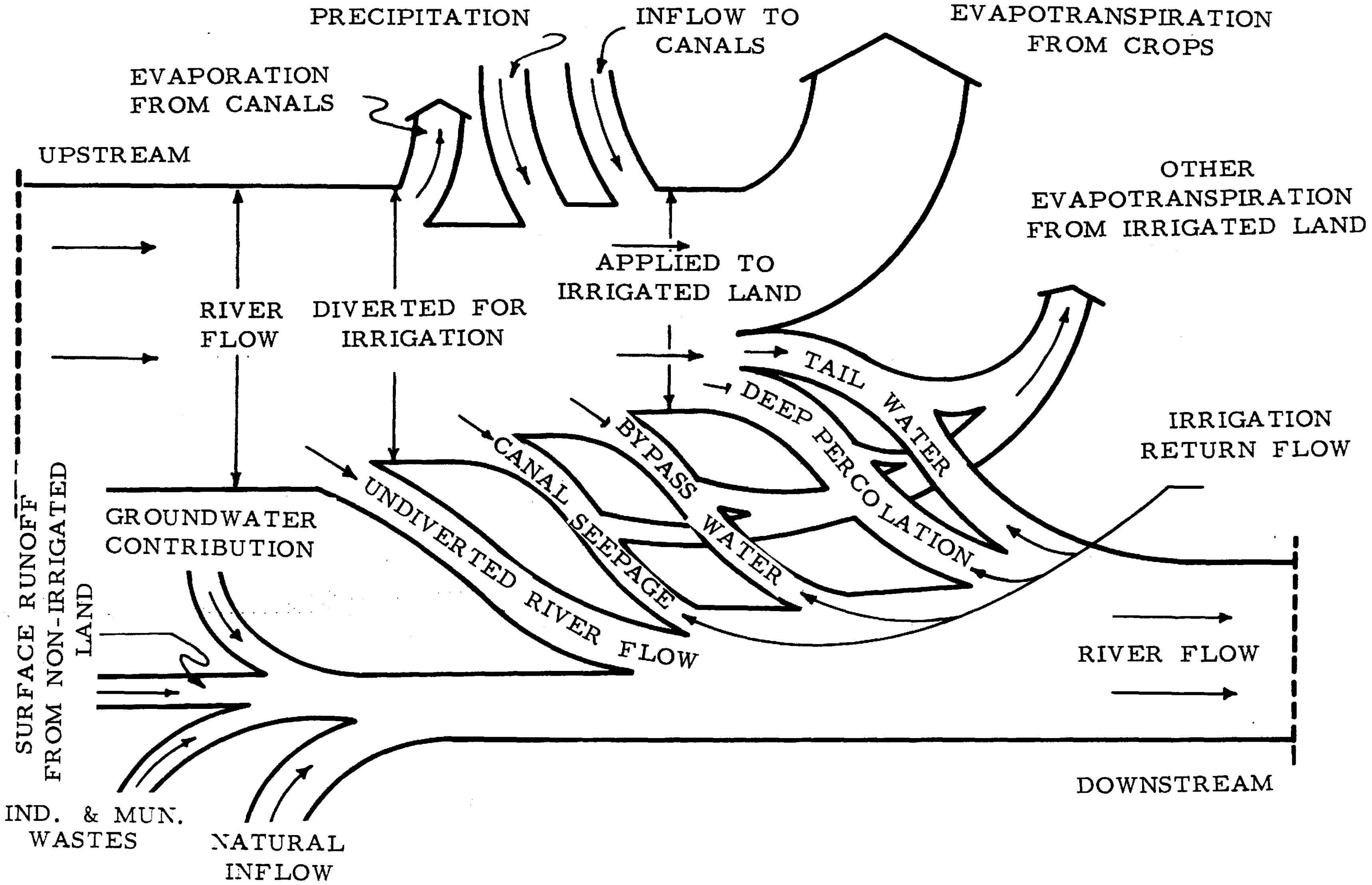


Figure 2. A typical irrigation return flow system (after Hornby, 1973).

Nitrogen Transformation Models

General

Development of a mathematical model of nitrogen transformations within a soil profile and linking it with a general hydro-quality system model requires pooling of knowledge from more than one discipline. Various soil scientists have studied the complex reactions not only between the cations and anions in solutions, but also between dissolved quality constituents and the soil and the use of these constituents by the crops.

Many authors, including Broadbent (1958 and 1966), reported valuable experimental data on the individual pathways of nitrogen transformations. Kirkham (1954, 1955), McLaren (1969, 1971) and a few others have formulated mathematical relationships for some of these transformation processes. Relatively few authors, including Dutt (1972), considered a majority of the nitrogen transformations in terms of a mathematical model.

Model of hydrolysis of urea

Fertilizer application contributes significant quantities of N to the soil. One of the forms in which N is applied is Urea, which initially undergoes hydrolysis in the soil water system. Broadbent, et al. (1958) and Overrein and Moe (1967) have conducted laboratory experiments and presented data on the factors affecting the hydrolysis of Urea. Shaffer et al. (1969) utilized these important kinetic factors and evolved a urea hydrolysis rate equation based on statistical regression analysis. Temperature and concentration of Urea-N were the variables considered in the equation.

Aviva Hadas and Kafkafi (1974) considered the slow-releasing nitrogen fertilizer "Improved Ureaform," and developed the kinetics of mineralization as influenced by temperature. The authors assumed first order reactions of the Michaelis-Menton type and evolved the rate constants which increased with temperature.

Mineralization and immobilization models

Kirkham and Bartholomew (1954 and 1955) derived theoretical equations for determining rates of mineralization and immobilization of plant nutrients in soil. The authors conceived a gross model represented by Figure 3. The model assumed the following first order rate equation for the net rate of change of available nitrogen atoms.

$$\frac{dx}{dt} = m - i \qquad \ldots\ldots\ldots \qquad (2.1)$$

in which

t = time

m = mineralization rate

i = immobilization rate

x = mass per unit mass of soil, of all available atoms, tagged and untagged.

The following assumptions were made in solving equation (2.1).

1. Heavy and non-heavy atoms behave the same in the soil.

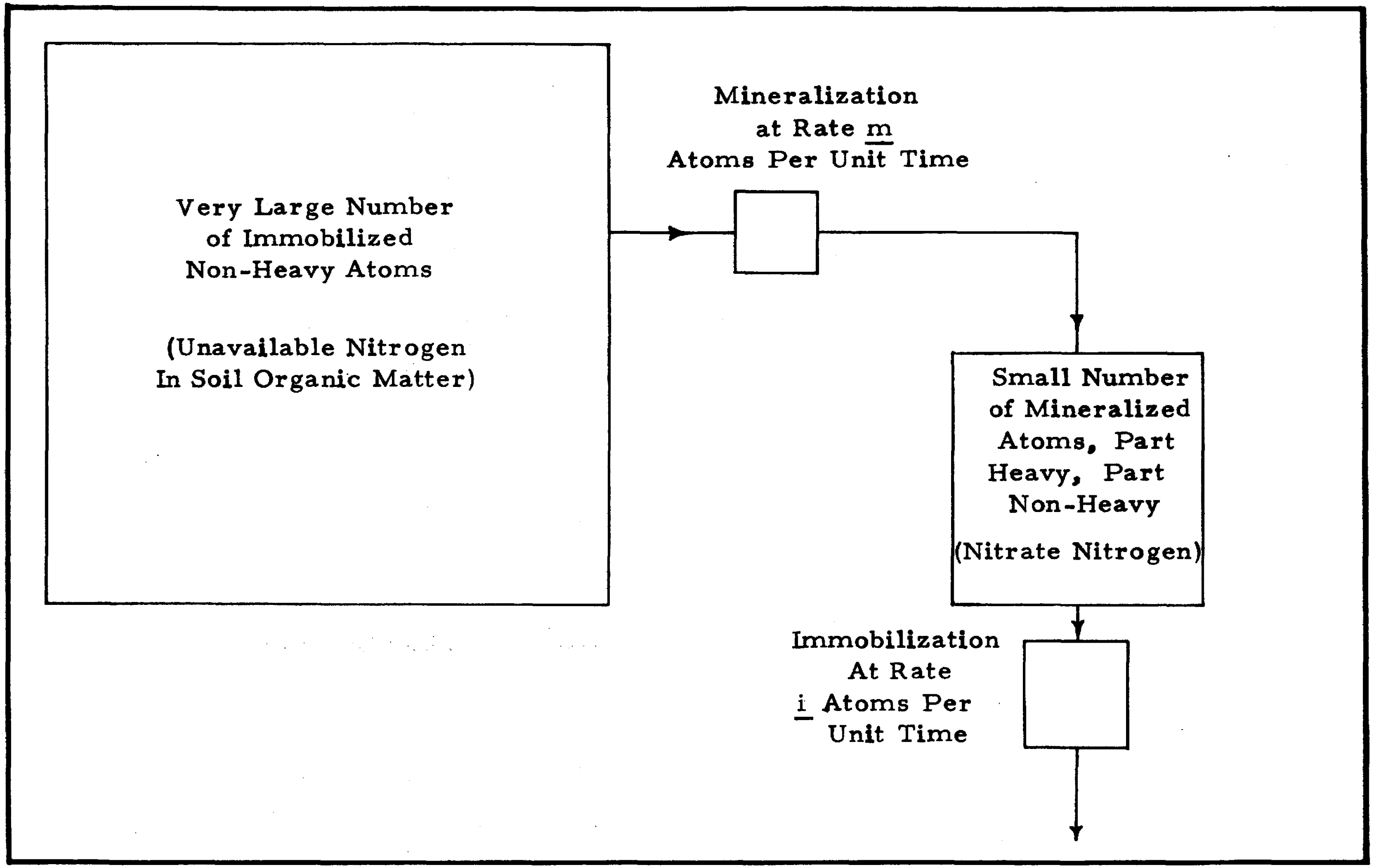


Figure 3. Representation of nitrogen transformation in soil. (After Kirkham and Bartholomew, 1954.)

2. Mineral atoms are so few in number ($\approx$ 100 pounds/acre) compared to the organic ($\approx$ 3000 pounds/acre), that the mineral atoms may be neglected as a source of mineralizing material, once they are immobilized.
3. The rates of mineralization and immobilization are constant during the time interval between successive measurements.

Broadbent and Tyler (1962), and Broadbent (1966) have studied the interchange between inorganic and organic N in soils. The experimental data indicated that both quantity and rate of N interchange depend not only on the earlier C:N ratios, but also on temperature, kind of inorganic N, activity of nitrifying bacteris, nature of clay minerals, and other soil factors. Shaffer et al. (1969) utilized these experimental data and evolved a rate equation for transformation using statistical regression analysis. The variables considered in this equation were temperature and concentrations of organic N, and ammonia-N.

Effect of temperature on soil nitrogen mineralization: Stanford and Smith (1972) concluded that cumulative N mineralized over time conformed to the first order rate equation:

$$\log (No - Nt) = \log No - \frac{k}{2.303(t)} \quad . \quad . \quad . \quad . \qquad (2.2)$$

in which

No = potentially mineralizable N

Nt = N mineralized in time, t (weeks)

k = mineralization rate constant, per week

The equation (2.2) gave best fit results for Portneuf silt loam soils (the soil classification for the area in this study). Stanford et al. (1973) proposed the following modified form of the Arhenius equation to represent the relation between temperature and mineralization rate applicable over a wide range of soil classification .

$$\log k = \log A - \frac{B}{T} \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (2.3)$$

in which

A = a constant

B = slope of regression

T = absolute temperature

and k is as defined in equation (2.2).

After substituting the derived values for the constants, the final equation is as follows:

$$\log k = 7.71 - \frac{2758}{T} \quad . \; . \; . \; . \; . \; . \; . \; . \quad (2.4)$$

in which T is defined in equation (2.3).

Nitrification models

This pathway of the transformation received maximum attention of many researchers. The kinetics of transformations are described by many authors assuming both the steady state systems and systems approaching steady state. Mathematical analysis and experimental data are available in the literature.

Steady state models

McLaren (1969a) set up an equation for steady state nitrification considering an open soil system. The basic nitrification reaction considered is as follows:

$$NH_4^+ \xrightarrow[k_1]{} NO_2^- \xrightarrow[k_2]{} NO_3^- \quad . \; . \; . \; . \; . \; . \; . \; . \; . \quad (2.5)$$

in which

k_1 = specific reaction rate for oxidation from NH_4^+ to NO_2^-

k_2 = specific reaction rate for oxidation from NO_2^- to NO_3^-

The bacteria responsible for rates k_1 and k_2, respectively, are Nitrosomonas and Nitrobactor. In deriving the rate constants the following assumptions were made.

1. The reaction rates could be considered as first order with respect to nitrite or ammonium concentrations provided these concentrations are not too high, in the consecutive sequence $NH_4^+ \rightarrow NO_2^- \rightarrow NO_3^-$.
2. It was assumed that the supply of oxygen is kept in excess, so as to be at constant activity.
3. The specific reaction rates k_1 and k_2, respectively, also depend on concentrations of enzymes responsible for the respective reactions, and these concentrations might be taken as proportional to the numbers of respective organisms present (Monod 1942, McLaren 1963).

Since the rate of nitrification (or nitrate accumulation in soils) depends on many environmental factors, such as temperature, pH, organic matter, and nitrifier population, Sabey et al. (1969) suggested use of delay rate to account for these factors. The authors postulated the following equation:

$$N = K_f R_k (t - t_f r_t) \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; (2.6)$$

in which

N = amount of NO_3^- - N in ppm accumulating in time t

K_f = characteristic nitrifying capacity in ppm NO_3^- - N/week (which would have to be determined from an incubation study). This is the maximum rate under optimum conditions.

R_k = (a fraction) a composite factor or index based on the relative maximum NO_3^- - N accumulation rates under less favorable conditions of moisture, temperature, pH, texture, aeration, etc.,

t = time in weeks from the date of ammonium application,

t_f = characteristic delay period under given nearly optimum conditions, and

r = (usually greater than one) index based on the relative delay periods under less favorable conditions.

Bazin and Saunders (1973) conducted further investigations to study quantitatively the consecutive oxidation of ammonium to nitrite and nitrate, and proposed a more general model of the open system. The best fit model proposed by Bazin and Saunders assumed that growth of the organisms could be described by a modification of the Verhulst-Pearl logistic equation, with the assumption that available particle surface area (or nutrient in some cases) limits the growth.

Effect of temperature on nitrification: Sabey et al. (1969) reported that actual rate of NO_3^- - N accumulation increased five times with 10 - degree temperature increase in some soils, while in others the change in actual rate was less than double with the same temperature increase. Knowles et al. (1965) used an electronic computer to integrate the simultaneous differential equations (Michaelis type) for bacterial growth, and thus determined the growth rate constants, saturation constants, and initial numbers of bacteria. These studies indicated a large temperature coefficient for growth rate constant for both nitrosomonas and nitrobactor species.

Non steady state models

Usually the time taken to reach the steady state in soil is typically of the order of one to two weeks and one would not normally expect more or less continuous rain for such a long period of time.

McLaren (1969b) proposed mathematical equations based on experimental work for nitrification. These equations are essentially for an open system with a constant rate of entry of a solution of ammonium, for concentrations of ammonium ions as functions of time of flow and distance within a soil column.

Saunders and Bazin (1973) disagreed with the mathematical analysis of McLaren (1969b) and proposed another generalized model shown by the following equation:

$$\frac{\partial s}{\partial t} + f \frac{\partial s}{t} = Q \quad . \; . \; . \; . \; . \; . \; . \; . \quad (2.7)$$

in which

Q = chemical reaction term

S = concentration of solute

f = flow rate

t = time

The assumption made in formulating equation (2. 7) are the following:

1. There is neither dispersion nor hydrodynamic diffusion.
2. Oxygen and other metabolites are present in excess.
3. Wastes are disposed of sufficiently efficiently so as not to poison the organisms.
4. The transformations are of first order with respect to ammonium and nitrite concentrations.
5. The specific rates of reactions are proportional to the biomass densities of the relevant organisms.

Biological oxidation of ammonium has been simulated in laboratory batch cultures under controlled conditions by Ardakani et al. (1974).

The concentration profiles are described by a modified Michaelis-Menten equation. Rate constants for oxidation of NH_4^+ to NO_2^- and NO_2^- to NO_3^- are 2.5×10^{-3} and 0.6×10^{-3} ppm/hour. cm^3 of soil per bacterium, respectively. Misra et al. (1974) have also found similar differences in the two rates. The values of the rate constants calculated from the field data are reported to be in good agreement with those obtained under controlled laboratory conditions. The authors suggested that these oxidation rate constants could be used for predictive modeling of soil inorganic nitrogen transformation.

Broadbent et al. (1957) conducted studies on nitrification of ammonical fertilizers in some California soils and reported that most rapid and maximum nitrification rates were attained under optimum conditions. Justice and Smith (1962) studied nitrification of ammonium sulphate in calcarious soils as influenced by combinations of moisture, temperature and levels of added nitrogen. Shaffer (1969) utilized the experimental data reported by Broadbent et al. (1957) and Justice and Smith (1962), and developed a rate equation for nitrification based on multiple regression analysis. The variables considered in the equation were temperature and concentrations of ammonia nitrogen and nitrate nitrogen.

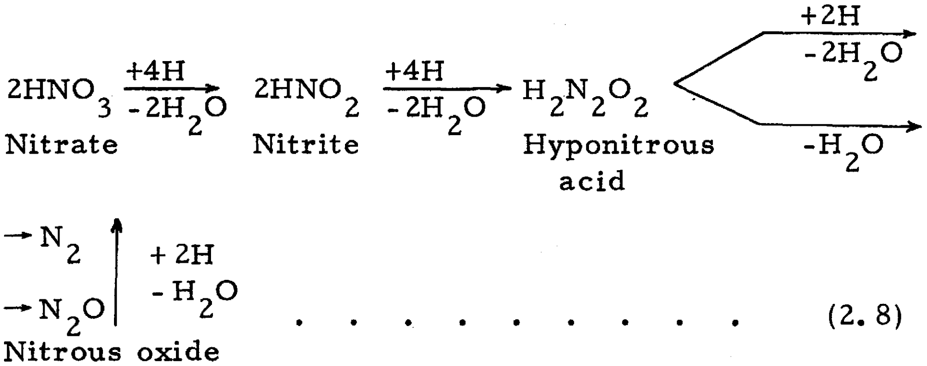
Nitrate immobilization models

One of the important pathways nitrate can take is the conversion of NO_3^- - N to microbial cell material at C:N ratios greater than about 23. Broadbent (1966) conducted experiments with tagged calcium nitrate as source of nitrogen for organisms decomposing added straw. The results evidenced the incorporation of some tagged nitrate with the organic fraction. Shaffer et al. (1969) utilized the experimental data of Broadbent (1966) and derived a rate equation for nitrate immobilization. The variables included in this equation are temperature and concentrations of organic -N and NO_3^- - N.

Denitrification models

Many authors, including Starr et al. (1974), reported that during continuous unsaturated leaching in a soil column there would be simultaneous occurrance of nitrification and denitrification. Denitrification occurs when soils become water-logged and anaerobic conditions prevail, so that the anaerobic organisms have the ability to obtain their oxygen from nitrates and nitrites. Gaseous nitrogen and nitrous oxides are the end products of denitrification.

The probable pathways whereby these losses come about are schematically indicated in the following equation (Tisdale and Nelson, 1966):



. . . . (2.8)

Starr et al. (1974) considered molecular diffusion together with sources and sinks under gaseous phase. One dimensional equation of the Ficks Law type is proposed as shown below:

$$q = -D\left(\frac{\partial C}{\partial x}\right) \text{ for steady state conditions} \quad . \quad . \quad . \quad (2.9)$$

and

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + F(x,t) \text{ for non steady state conditions} \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (2.10)$$

in which

q = steady state rate at which a particular gas diffuses.

D = apparent diffusion coefficient (assumed constant for a given soil-water content), cm/day

C = concentration of nitrogen compound in soil solution

$F(x,t)$ = a source (production) term if it is positive in sign and a sink (consumption) term if negative

x = distance within soil

t = time

The conclusion arrived at by Starr et al. (1974) is that most of the oxygen removal takes place within the top 10-20 cm of soil, and below a depth of about 30 cm the oxygen level remains nearly constant. In the combined model developed by Dutt et al. (1972), gaseous losses of nitrogen were assumed to be negligible, as aerobic conditions were assumed to exist predominantly. Further discussion on denitrification is, therefore, beyond the scope of the objectives and is not reviewed further.

Combined Transformations Models

Kinetic approach was adopted in evolving a combined model incorporating all the pathways of nitrogen transformations because the reaction times involved in these transformations are of the order of days or weeks.

Dutt et al. (1972) developed a mathematical model of nitrogen transformations and incorporated it into a chemical model of soil and water system. The following pathways of transformations were considered in the model.

1. Hydrolysis of Urea.
2. Nitrogen immobilization and mineralization.
3. Nitrification.
4. Nitrate immobilization.

The rate equations were those developed by Shaffer et al. (1969) based on linear regression analysis of observed experimental data reported by various authors, including Broadbent et al. (1957), Overrein and Moe (1967), and Broadbent (1957, 1966). The combined model successfully predicted the concentration of nitrate reaching an unfluctuating water table below the root zone. Included in this model is a factor for uptake of nitrogen by growing crops.

Endelman et al. (1972) applied a systems analysis approach to terrestrial nitrogen cycle. They used the conservation of mass principle to provide a theoretical basis for developing the systems mathematical model. The rate equations for biological transformations of nitrogen are based on linear regression of literature data for immobilization and on Michaelis-Menten type equations for nitrification. The authors feel that the approach is more sophisticated and can yield more refined simulation than that achieved by Dutt et al. (1972).

Ferrari and Cuperus (1973) have developed a simulation model of leaching non-adsorbed anions with special reference to nitrate. The model assumes that transport of ions is only caused by mass flow and hydro-dynamic dispersion, neglecting the effects of diffusion. The model, however, does not consider the biological transformation of nitrogen within the soil profile, and can compute the leaching or accumulation of nitrate or chloride essentially at or above the groundwater table.

Inasmuch as it is theoretically sound and adopted in soil-water systems, the biological transformation model and its incorporation in a general hydroquality model will form an important segment of this modeling task (see Chapter IV).

CHAPTER III

GENERAL HYDRO-QUALITY MODEL

Introduction

Systems approach is followed in formulating and analyzing the problem of predicting the quality of return flow. Since the quality of irrigation return flow is affected by chemical and biological changes during an irrigation cycle, a gross conceptual model representing the basic structure of this hydrologic-chemical-biologic cycle of the overall system (Figure 2) is shown by Figure 4. Described herein are the computer simulation models of the three subsystems envisioned in the conceptual model. The various processes considered in developing the overall computer model are the following:

1. Precipitation.
2. Snowmelt.
3. Evapotranspiration.
4. Surface water and groundwater movement.
5. Chemical changes of percolating water.
6. Biological processes to include microbial nitrogen transformations.
7. Nitrogen uptake by crops and other aquatic biomass.
8. Mixing of irrigation return flow with surface and groundwater.

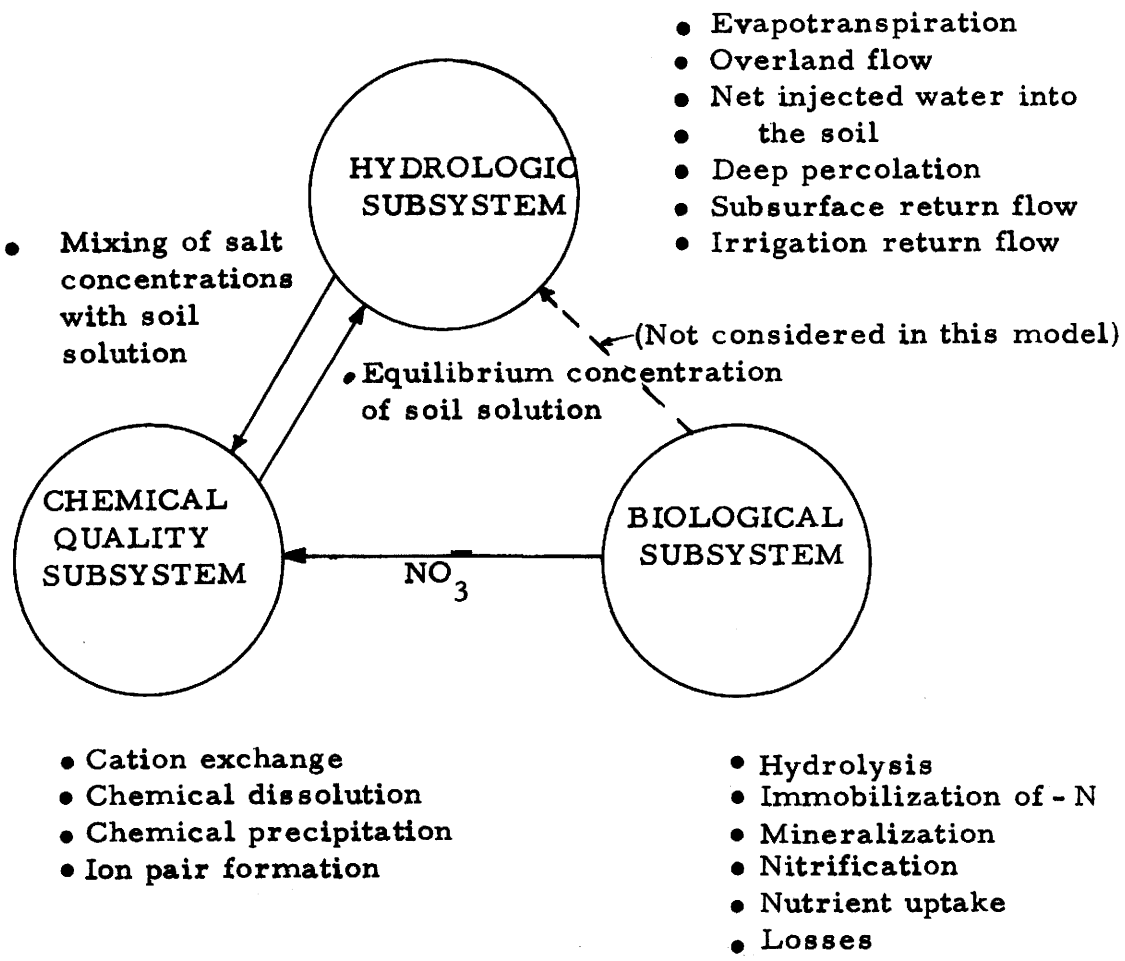


Figure 4. A conceptual model of an irrigation return flow system -- component subsystems and linking processes.

The chemical and biological simulation models have essentially been developed utilizing techniques similar to those adopted by Thomas et al. (1971) and Dutt et al. (1972). Theoretical considerations in developing these biological simulation model, however, are included in Chapter IV.

Hydrologic Subsystem Simulation Model

The hydrologic portion of the model simulates the mathematical descriptions of the various hydrologic processes. The continuity of mass principle links the individual processes into a system simulation model. The general model developed in the present study is adopted from the works of Thomas et al. (1971) and Hill et al. (1973). Particular changes applicable for a typical irrigated area are found in representing the water conveyance and/or irrigation efficiencies, and in the subsurface return flows.

The basic mathematicalmodel of a hydrologic system is represented by the following continuity equation:

$$\text{Inflow} - \text{Outflow} = \text{Change in storage} \quad \ldots\ldots\ldots \quad (3.1)$$

A conceptual model of the various hydrologic processes shown by Equation (3.1) is based on Hill et al. (1973) and is given in Figure 5. Each block and the connecting line are represented mathematically in the model.

A more explicit representation of Equation (3.1) for simulation purposes is described by Wang et al. (1973) and is expressed by Equation (3.2):

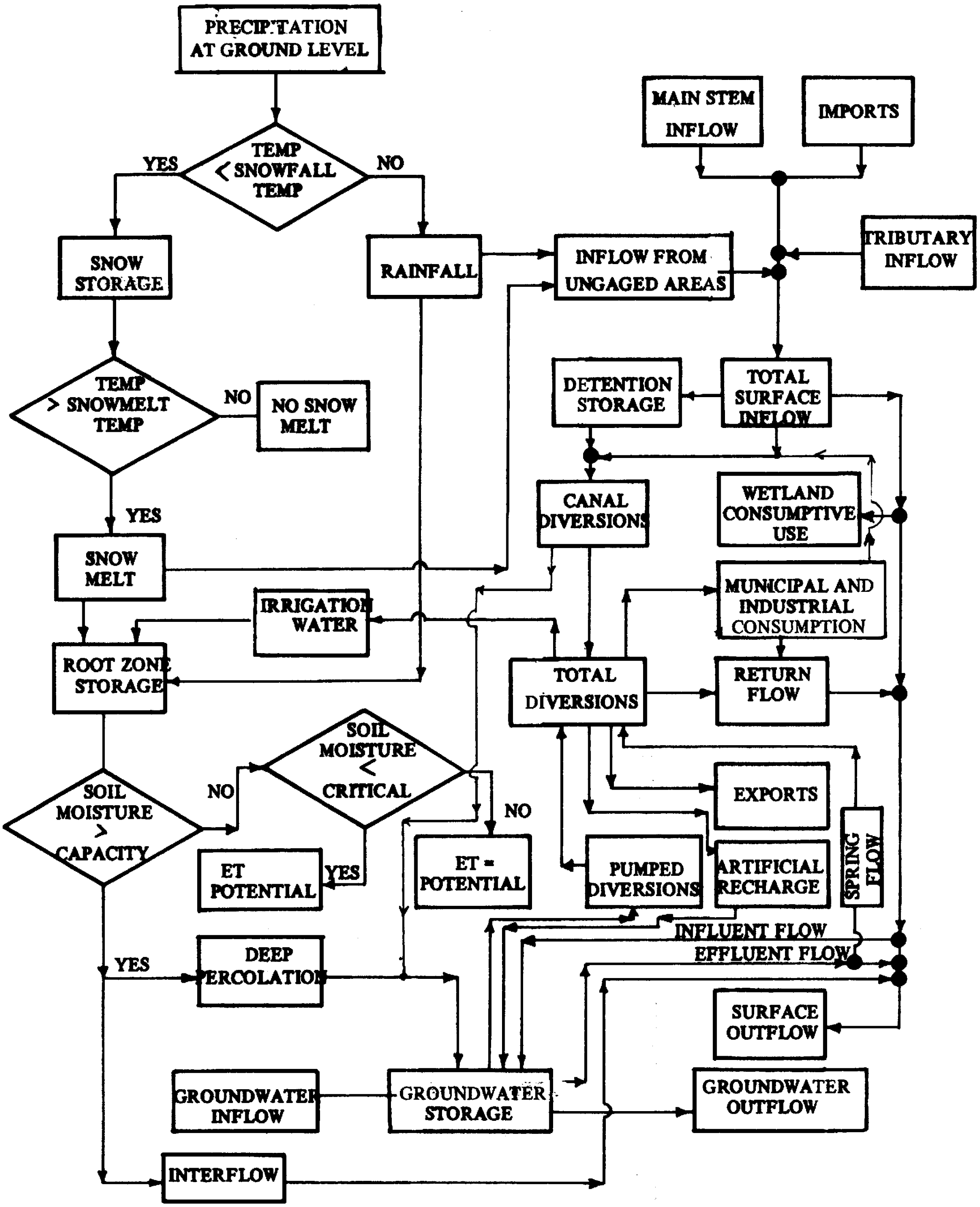


Figure 5. Schematic diagram of hydrologic model.

$$Q_{so} = Q_{si} + Q_{ri} + Q_{rmi} + Q_{bf} - W_{sd} - W_{smi}$$

$$+ W_{ii} + W_{imi} - W_x + ds \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (3.2)$$

in which

Q_{so} = surface outflow from the basin

Q_{si} = surface inflow in streams

Q_{ri} = irrigation overland and interflow

Q_{rmi} = municipal and industrial return flows

Q_{bf} = base flow

W_{sd} = surface diversions for irrigation

W_{smi} = municipal and industrial diversions from surface supplies

W_{ii} = imports for irrigation

W_{imi} = municipal and industrial imports

W_x = exports

ds = change in surface storage within the basin (increase in ds being assigned a negative value)

For modeling purposes the Equation (3.2) is further refined to suit the study area and is written as:

$$\text{SUMOUT (I)} = \text{SRF (I)} + \text{SNPC (I)} + \text{STRC (I)} +$$

$$\text{GWBF (I)} + \text{SUBSRF (I)} \quad . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \; . \quad (3.3)$$

in which

I = time interval under consideration (one month in this model)

SUMOUT = total surface runoff

SRF = direct runoff from surface channels

SNPC = ungaged runoff correlated to precipitation and snowmelt

STRC = ungaged runoff correlated to canal diversion

GWBF = routed ungaged influent subsurface flow correlated to precipitation and snowmelt

SUBSRF = quantity of routed deep percolation appearing as surface runoff

The modeling procedure involved solving Equation (3.3) for SUMOUT (I), the total surface runoff. The quantities on the right hand side of Equation (3.3) are calculated as described by the following equations:

$$SRF\ (I) = [1 - EFF(I)]\ Qr\ (I) \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (3.4)$$

in which

EFF(I) = proportion of water, Qr(I), applied to land including crop requirements and canal seepage. This includes both conveyance and application efficiencies

Qr(I) = quantity of canal diversion

$$SNPC\ (I) = C_1\ (PRE + SNMLT - C_2) \quad . \quad . \quad . \qquad (3.5)$$

in which

PRE = precipitation

SNMLT = snowmelt

C_1 and C_2 are constants

$$\text{STRC (I)} = C_3\,(\text{Qr(I)} - C_4) \quad \ldots\ldots\ldots \quad (3.6)$$

in which

C_3 and C_4 are constants

$$\text{GWBF (I)} = C_5\,(\text{PRE} + \text{SNMLT} - C_6) \quad \ldots\ldots \quad (3.7)$$

in which

C_5 and C_6 are constants

$$\text{SUBSRF (I)} = \text{FK (I) (ARF)} \quad \ldots\ldots\ldots \quad (3.8)$$

FK (I) is the fraction of routed subsurface return flow contributing to surface runoff.

ARF = average value of routed subsurface return flows of the previous and the current time increments.

In the above equations, the constants C_1, C_2, C_3, C_4, C_5, and C_6 have been verified through modeling procedure and proved adequate for the study.

Having known all the quantities on the right side of Equation (3.3) represented in the model by measured inputs or mathematical functions, it is possible to calculate the outflow from the watershed and compare the computed value with the observed value. Many parameters are assumed initially and calibration of the model consisted of systematically varying the parameters till the model represents the observed outflow of the specific prototype hydrologic basin over a specified period of time.

Capabilities of the Hydrologic Model

After combining different characteristics of the models developed by Thomas et al. (1971) and Hill et al. (1973), the final model of the subsystem has the important capabilities suitable to the particular irrigation system investigated. Some of the more important capabilities are listed below:

1. Data reduction program which inputs raw data and arranges it into the proper order and location for use by the basic models.
2. Calibration algorithm which controls the hydrologic submodel during the parameter selection process. In this process, monthly output values determined by the model are compared with actual recorded values, and the parameters which produce an acceptable match between the observed and computed data are identified.
3. Incorporating time variant parameters for the following:
    - a. Water application and/or conveyance efficiencies.
    - b. Fraction of subsurface return flow contributing to surface runoff.
4. Linking of the hydrologic and chemical quality models to produce the hydro-quality model.

Chemical Quality Subsystem Simulation Model

The general principle followed in water quality modeling is that each component portion of the surface runoff described by Equation (3.3) has a measurable quantity of quality parameter. Identification and prediction of this quality component will describe the quality of return flow. Since the return flows consist of surface and subsurface components, a prediction model needs to consider the quality changes that occur in both these components of return flows. In an irrigation system, however, the overland portion of return flow normally differs little in chemical composition from that of the applied water because of limited contact with soil. Neglecting the pickup of impurities like fertilizers, pesticides, organic matter, sediment, and debris, the chemical quality model envisioned in this study, therefore, considers the major changes in the quality of applied water as it passes through the soil profile.

Represented by Figure 6 is a block diagram of the conceptual model of the subsystem. Concentration of a water quality constituent in any segment within a layered soil system has been described by Tanji et al. (1967a, 1967b) as shown in the following equation.

$$C_i = C_{i-1}\left[\frac{PV_i - FM_i}{PV_i}\right] + C_i^o\left[\frac{FM_i}{PV_i}\right] \quad . \; . \; . \; . \; .(3.9)$$

in which

i = segment number of a soil profile

C = concentration of a solute species

PV_i = saturated pore volume of segment i

Legend:

N = Number of soil layers
DP = Depth of deep percolation water
Q = Aliquot depth = DP/N
PV_i = Pore volume of soil layer i
FM_i = Field moisture content of layer i
C_i = Concentration of species in the ith layer

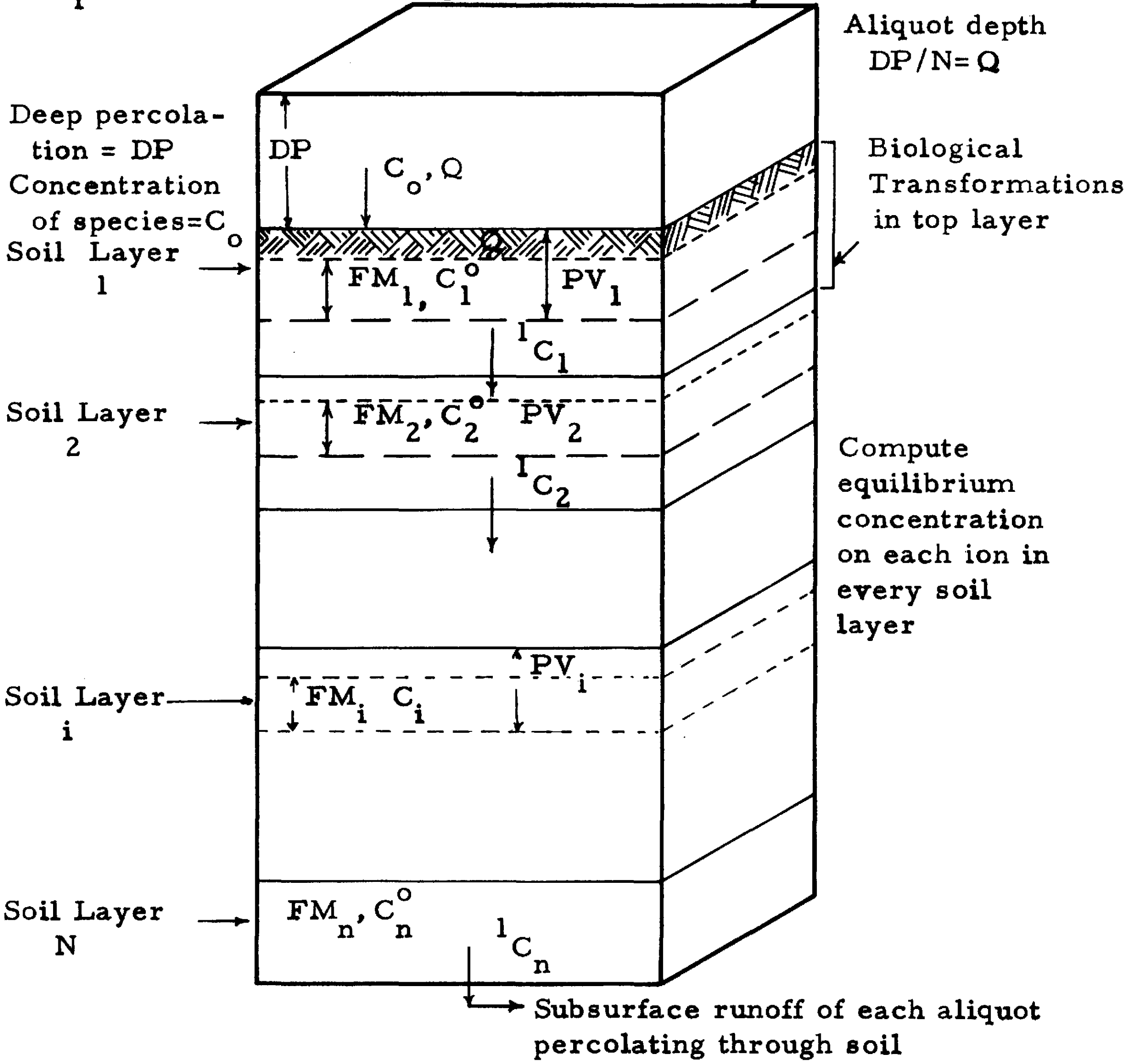


Figure 6. Conceptual model of chemical quality subsystem.

FM_i = field moisture content of segment i

C_i^o = initial concentration of C at field moisture content.

The underlying assumption in deriving the Equation (3.9), however, is that water movement takes place when the pore spaces in the soil are completely filled with water. For modeling purposes, therefore, the concentration of a quality constituent of subsurface return flow can be represented by the average concentration of water leaving the last segment at the bottom of soil profile. This can be represented by the following equation:

$$C_{Ii} = \left[\frac{1C_n + 2C_n + \ldots + {}^{m}Cn}{m} \right] \quad . \quad . \quad . \quad . \quad . \quad . \quad (3.10)$$

in which

m = number of aliquots of applied water (deep percolation)

n = number of soil layers considered in the model

C_{Ii} = average concentration of a solute species i comprising the subsurface return flow in time increment I

$1C_n$ = concentration of 1st aliquot after percolating through n layers of the soil

${}^{m}Cn$ = concentration of m^{th} aliquot after percolating through n layers of the soil.

The quantity of ${}^{m}Cn$ is computed each time from Equation (3.9).

The modeling procedure involved in solving Equation (3.10) for C_{Ii}, the concentration of a solute species comprising the subsurface return flow. Each component of the right hand side of Equation (3.10) will have to be computed taking into consideration the various chemical reactions involved for attaining an equilibrium concentration of the solute species within the soil water system of the segments under consideration. The total quantity of a solute species in the subsurface component of return flow is obtained by the following equation:

$$Qi = C_{Ii} \cdot \text{SUBSRF (I)} \cdot \text{CONV} \quad . \quad . \quad . \quad . \quad . \quad . \qquad (3.11)$$

in which

Qi = quantity of a solute species i comprising the subsurface return flow, say, in tons

CONV= a conversion factor

SUBSRF (I) and C_{Ii} are as defined in Equations (3.8) and (3.10), respectively.

The accuracy of the total quantity of a solute species (ion), therefore, depends upon the nature and extent of ions describing the soil water system. The specific solute species considered in this chemical quality model are Ca^{++}, Mg^{++}, Cl^{-}, Na^{+}, HCO_3^{-}, $SO_4^{=}$, and NO_3^{-}. The various chemical reactions involving these ions are developed by Dutt et al. (1972) and are shown by Figure 7. These chemical reactions are based on equilibrium concepts and solubility product principles. Theoretical considerations in developing these equations have been adequately described by Dutt et al. (1972). A discussion on the theoretical development of the equations is shown by Appendix A .

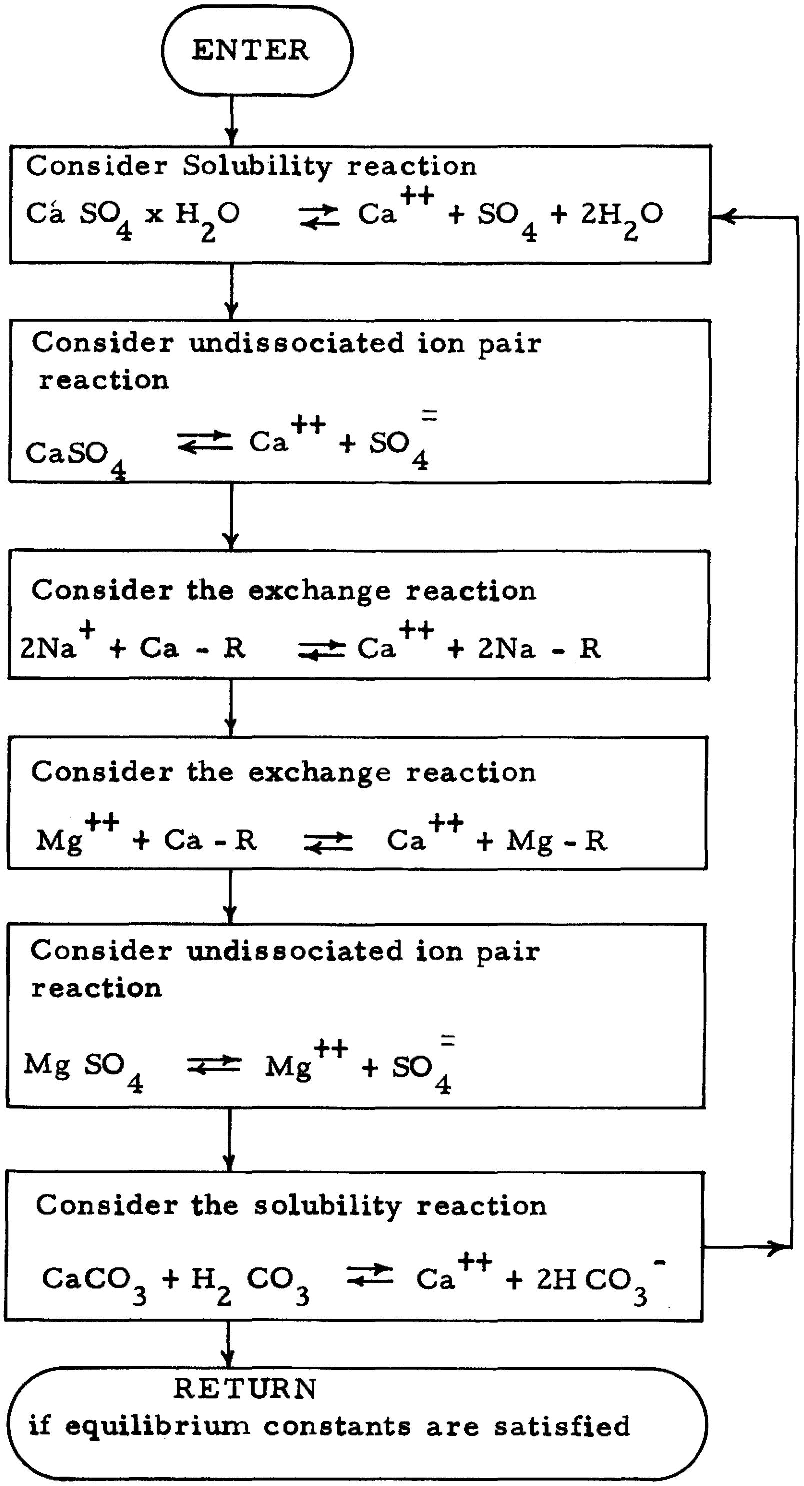


Figure 7. Block diagram of chemical reactions considered in the chemical quality model.

The chemical quality model described above follows the general principles adopted by Thomas (1971) and incorporates the improvements suggested by Dutt et al. (1972). Described herein are the more important improvements in the chemical quality model adopted in this study.

A technique to represent more exactly the true ionic concentration of initial soil colution is necessary for the following reasons:

1. Several authors, including Woolhiser (1973), have indicated that, unlike in hydrologic modeling, the initial concentrations are particularly important in the soil water system. It has also been verified in this study that the initial concentrations of ions in soil solution serve as driving parameters for the chemical reactions and will effect the system for a long time.
2. Utilizing the concept of ion pair formation, the desirability of correcting the measured ionic concentrations of soil solution extracts to their respective activities has been suggested by many authors, including Fred Adams (1971) and Dhanpat Rai and Franklin (1973).

The ionic concentrations of particular interest in terms of this model are those of the divalent cations and the sulphate ion. The true concentrations of each of these ions can be represented as:

$$C_{Ca_t} = C_{Ca} + C_{CaSO_4} \quad . \; . \; . \; . \; . \; . \; . \; . \qquad (3.12)$$

$$C_{Mg_t} = C_{Mg} + C_{MgSO_4} \quad . \; . \; . \; . \; . \; . \; . \qquad (3.13)$$

$$C_{SO_{4_t}} = C_{SO_4} + C_{CaSO_4} + C_{MgSO_4} \quad . \quad . \quad . \qquad (3.14)$$

in which

C represents the concentration of the ion or the ion pair, while the suffix t represents the total concentration of the respective ion.

Since no reliable analytical methods to find the concentrations of exchangeable cations are available for calcarious soils (Dutt et al. 1972), these corrected ionic concentrations are adopted to compute the concentrations of exchangeable cations in order to predict the soil solute composition.

The computer algorithm based on the above principles has been verified by Dutt et al. (1972) and Gupta (1972). The inputs to the chemical quality model included the measured concentration of ions in gaged surface inflows, estimated concentrations of ions in ungaged inflows (both surface and subsurface), and measured or estimated concentrations of ions in the initial soil solution. The concentration of nitrate ion in the initial soil layer is, however, predicted from the biological transformations model.

Biological Transformation Model

In terms of prediction modeling a soil-water system is not adequately represented within the chemical quality subsystem without a proper evaluation and inclusion of transport of the essential nutrients through the soil-water system. Among the nutrients of major concern as pollutants are nitrogen and phosphorus. Pathways of movement of nitrogen in the soil profile and its accumulation in the groundwater are of concern in terms of pollution hazard of this nutrient. Phosphorus is, however, not considered in this endeavor because of the relatively lesser magnitudes both in terms of its concentration and pollution hazard of groundwater.

Nitrogen in the groundwater is a part of the overall nitrogen cycle. It can originate from the rain, soil, organic matter, manure, an accumulation in the soils prior to irrigation, fixed by microrganisms, fertilizers, and from the wastes in urban and industrial runoff. It is removed from the soils by crop uptake, denitrification, volatilization, and leaching through soil profile and in the drainage waters. The principal form nitrogen takes in the soil is the highly oxidized form of nitrate ion, which is water soluble and moves along with percolation water in the soil profile. The various oxidation levels of N in soil are brought about by biological transformations. The biolgical subsystem, therefore, considers the various nitrogen transformations and their interrelationships. A conceptual model is developed by Dutt et al. (1972) after combining the biochemical and chemical pathways within the soil. The model includes those nitrogen transformations which are performed biochemically by micro-organisms or chemically by nonbiological reactions.

Represented by Figure 8 is the conceptual model for the biological subsystem (Dutt et al. 1972). Nutrient transport within a soil -

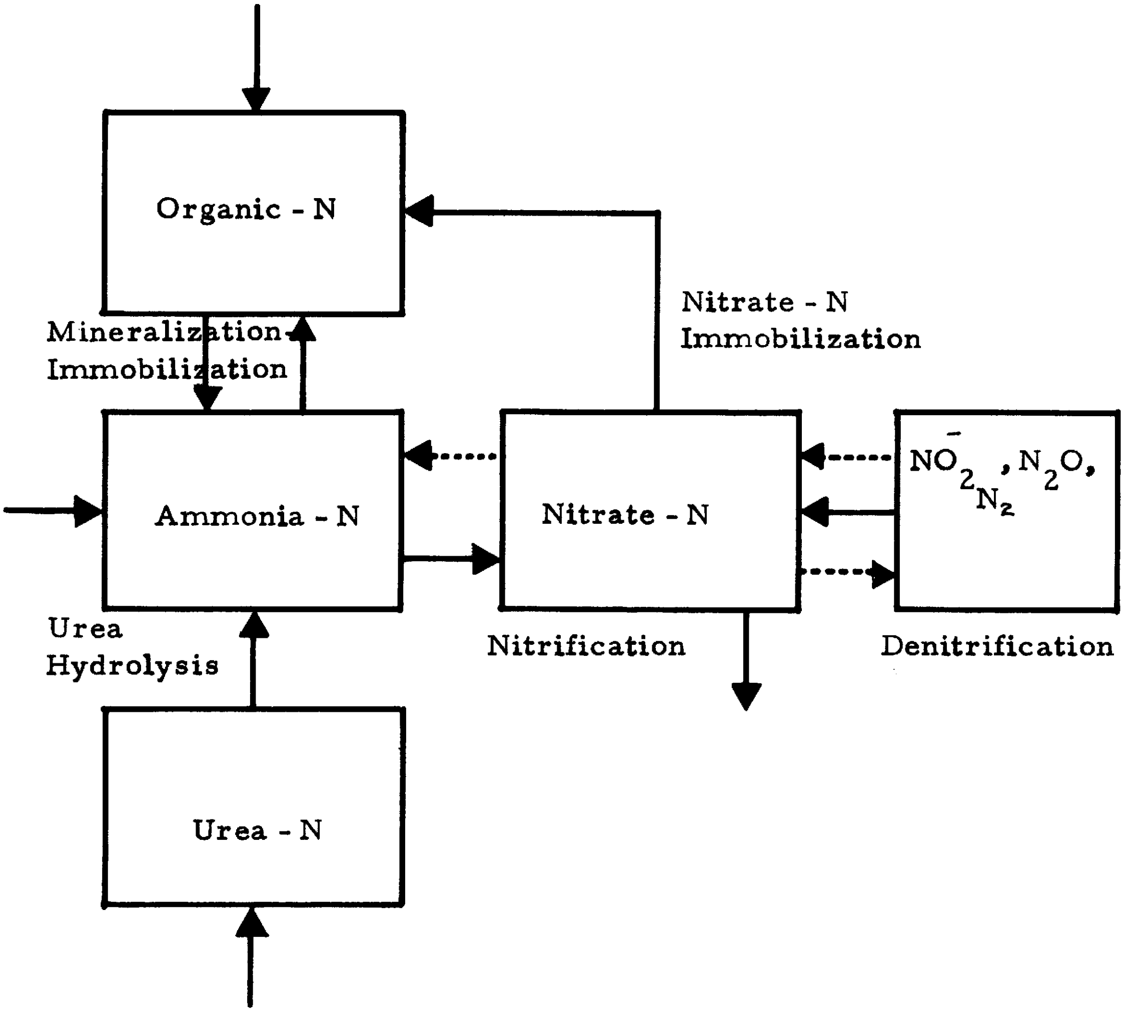


Figure 8. Biochemical and chemical pathways within the system model.

water system can be represented as follows. The continuity of mass for an elemental segment of a soil-water system can also be shown by Equation (3. 1) for a discrete time interval.

A more explicit transport equation developed by Endelman et al. (1972) is as follows:

$$\begin{bmatrix}\text{Rate of mass}\\\text{accumulation}\end{bmatrix} = \begin{bmatrix}\text{Rate of mass}\\\text{in}\end{bmatrix} - \begin{bmatrix}\text{Rate of}\\\text{mass out}\end{bmatrix} + \begin{bmatrix}\text{Net rate of appearance}\\\text{of mass by reaction}\end{bmatrix} \quad \ldots\ldots\ldots \qquad (3.15)$$

This is expressed as a partial differential equation as:

$$\frac{\partial(ec)}{dt} = \frac{-\partial(cv)}{z} + \partial\left[eD\ (\partial c/\partial z)\right] \partial z + \Sigma R_i \qquad (3.16)$$

in which

c = concentration of a nitrogen compound (NO_3^-) in a carrier (mass/unit-volume of carrier)

e = volume of carrier (water) per unit volume of soil

v = volume flux of a carrier (volume of carrier/unit cross sectional area of soil/time)

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

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

t = time

z = depth of soil column

Neglecting dispersion for a discrete time interval, the Equation (3.16) is represented for modeling purposes in this study by the following equation in respect of nitrogen accumulation within a soil profile.

$$\begin{array}{l} \begin{array}{c}\text{Mass of N at end}\\ \text{of time step}\end{array} = \begin{array}{c}\text{Mass of N at beginning}\\ \text{of time step}\end{array} + \\ \begin{array}{c}\text{Mass of N accumulated}\\ \text{within the time step}\end{array} - \begin{array}{c}\text{Mass of N uptake}\\ \text{by crop}\end{array} \\ - \begin{array}{c}\text{Other}\\ \text{Losses}\end{array} \quad \ldots\ldots\ldots\ldots \qquad (3.17) \end{array}$$

For modeling purposes Equation (3.17) is also written as:

$$AN_2 = AN_1 + AN - UPTK - LOSS. \quad . \quad . \quad . \qquad (3.18)$$

in which

the elements in Equation (3.18) have one to one correspondence with the elements in Equation (3.17).

The modeling procedure involves solving the above equation for AN_2, the mass of nitrogen at end of a time step. Each of the quantities on the right side of Equation (3.18) must be measured, calculated, or estimated in order to solve the Equation (3.18). Input quantities to the model are the following:

1. Chemical composition of surface application of fertilizers and organic matter turnover by the crops and their usual C:N ratio to facilitate calculation of nitrogen content at the beginning of a time step.

2. An estimate of quantities of nitrogen uptake by growing crops for the study area.

3. Mass of nitrogen accumulated within the time step AN is predicted taking the biological transformations of nitrogen within the soil profile. The following transformations are, however, considered:
    - a. Hydrolysis of Urea.
    - b. Mineralization and immobilization of organic nitrogen.
    - c. Nitrification of ammoniacal nitrogen.
    - d. Nitrate-N immobilization to organic-N.

Nitrogen compounds assumed in Equation (3. 18) are NO_3^- and NH_4^+, as these are the predominant inorganic forms that the crops can uptake. The quantity of nitrate ion present in soil solution is utilized by the chemical quality model to calculate the equilibrium concentrations of other ions from the increased ionic strength of soil solution.

The following assumptions are, however, made in the biological subsystem model.

1. Nitrogen transformations occur within the zone of root influence only.

2. Percolation is slow enough for equilibrium to be established in each soil stratum.

3. The behavior of nitrate is the same as that of a chloride ion, in that it is assumed to be a conservative parameter (does not enter into chemical or biological reactions).

4. No appreciable denitrification occurs below the root zone and within the groundwater system.

5. The rate of movement of NO_3^-, below the zone of root influence, is the same as that of water.

Linking of Chemical Quality and Biological Subsystems

The two models are linked together using the principle of similarity as "Conservative parameters" in respect to NO_3^- and Cl^- ions, as discussed herein.

Several authors, including Pratt et al. (1972), have measured the NO_3^- content within and below the effective rooting depth of crop to evaluate the loss of NO_3^- to the crop or for fertilizer management, and to study the leaching losses. Represented by Figure 9 are some typical distributions of NO_3^- within and below the root zone for a typical sandy loam type of soil. A similar distribution in respect of Cl^- ion is also shown by Figure 9. It is seen from Figure 9 that the fluctuations in the concentrations of NO_3^- are maximum within the root zone.

A majority of biological transformations are, therefore, assumed to occur within the zone of root influence. In terms of the general and gross nature of this modeling technique, however, the concentrations of nitrate is evaluated treating the entire depth of root zone as one layer. Thus, the computed concentration of nitrate is considered in the topmost layer of the soil profile for evaluating the ionic strength of soil solution for subsequent equilibrium calculations of various ions.

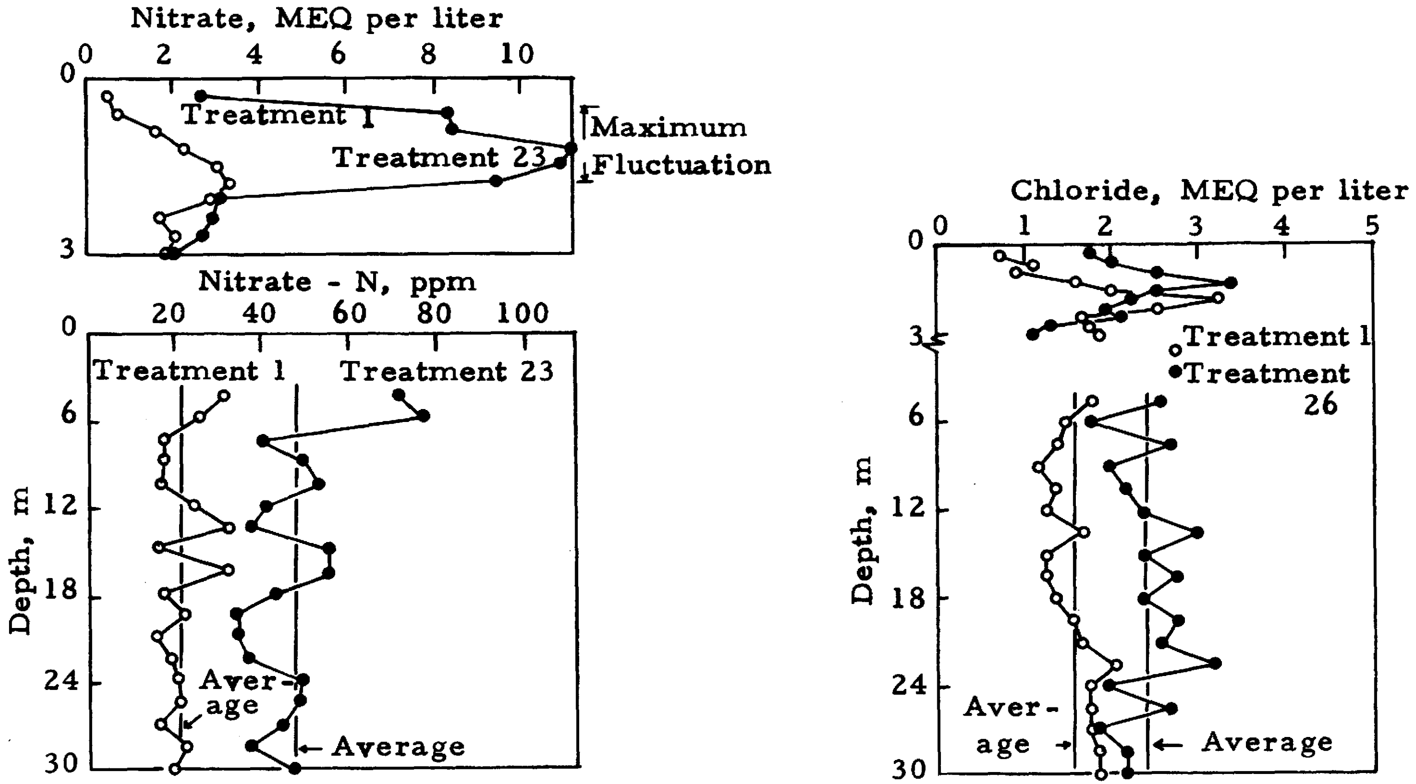


Figure 9A. Relationship between NO_3^- concentration in the saturation extract and depth (0 to 3 m) and between NO_3^- N concentration in the soil solution and depth (3 to 30 m) for two treatments.

Figure 9B. Relationship between Cl^- concentration and depth for two treatments. The top part is for saturation extracts and the lower part is for soil solutions.

Figure 9. Typical distribution of NO_3^- and CL^- within and below root zone. (After Pratt et al., 1972)

Assuming further that nitrate is a conservative parameter as a chloride ion, no biological transformations are assumed to occur in the subsequent layers of the soil profile. The modeling procedure involved in linking the biological and chemical models is, however, demonstrated in Figure 6.

Capabilities of the Combined Hydro-Quality Model

The combined model predicts the quantity and quality of the return flow from an irrigation system. The model operates on monthly time increments with a variable spatial resolution. The quality parameters considered in the model are Ca^{++}, Mg^{++}, Na^{+}, K^{+}, Cl^{-}, HCO_3^{-}, $SO_4^{=}$, and NO_3^{-}.

CHAPTER IV

THEORETICAL CONSIDERATIONS

Introduction

Theoretical considerations in developing the hydrologic and chemical quality models are adequately discussed in Chapter III. Modeling the biological subsystem takes the kinetic approach in the reaction times involved in nitrogen transformations. Described in this chapter are the theoretical considerations in developing the microbial nitrogen transformation model.

Nitrogen Transformations in Soil Profile

General

Before considering the necessary transformations of N in the soil profile, it is essential to consider the complexity of nitrogen in the soil water system. Transformations of nitrogeneous species can be illustrated by the overall nitrogen cycle shown by Figure 10 (Keeney and Gardner, 1968). Input of nitrogen to the soil can be grouped under precipitation, organic wastes and plant debris, fertilizers, and nitrogen fixed biologically, in addition to the existing nitrogen content of soil organic matter. Within the soil profile, nitrogen, which mostly occurs as a part of the soil organic matter complex, undergoes complex transformations between its various forms by means of chemical, physical, and biological processes.

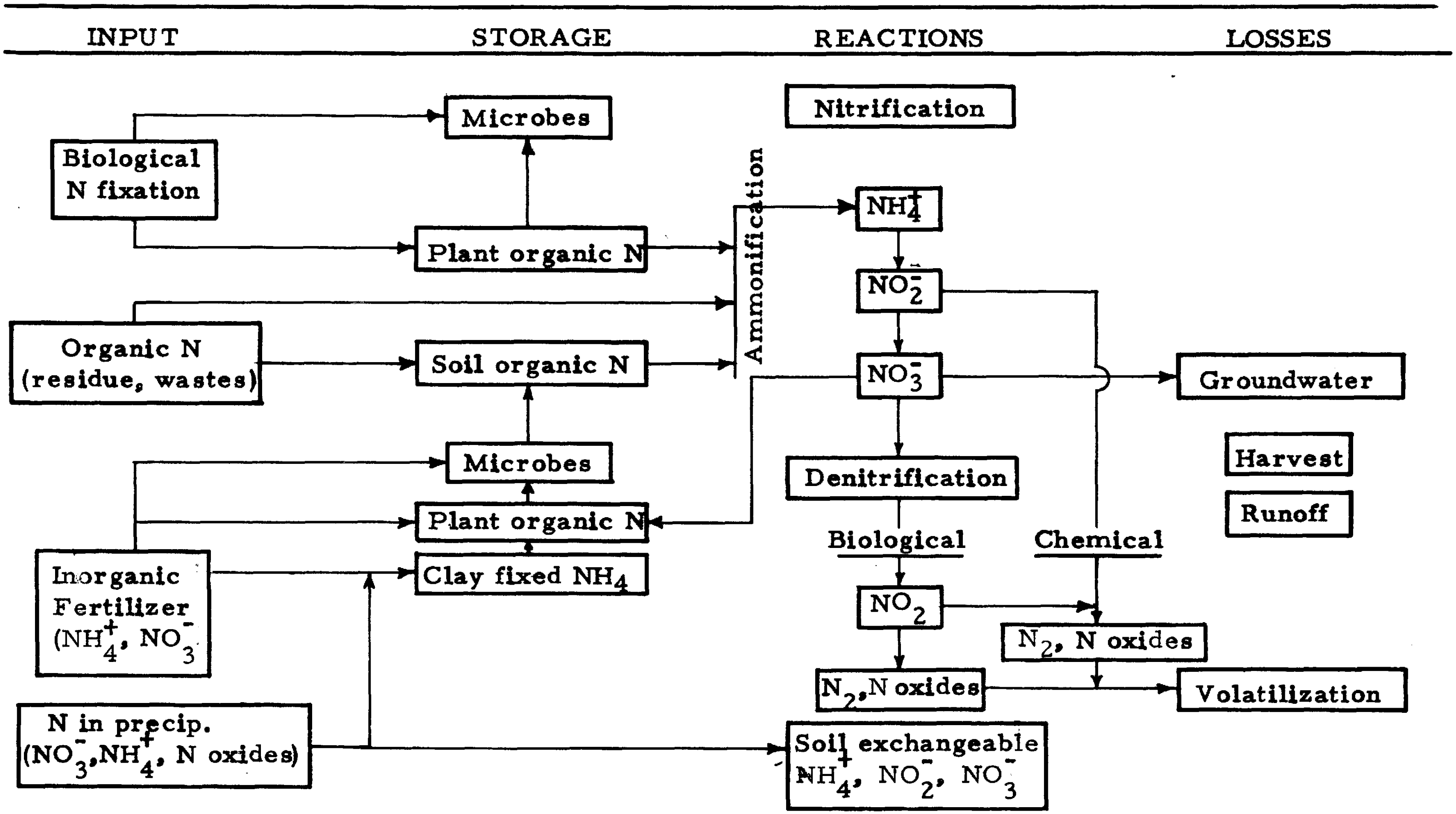


Figure 10. Detailed nitrogen cycle. (After Keeney, D.R., and W. R. Gardner, 1968.)

The complicated role of nitrogen within the plant-soil-water system with reference to its unusual number of oxidation levels or valences, is shown by Figure 11 (Delwiche, 1970). These oxidation levels explain the ability of nitrogen to combine with hydrogen, oxygen, and other atoms to form a great variety of biological compounds. It is, therefore, important to consider the various pathways and kinetics of formation of these compounds to estimate the available forms of nitrogen, the inorganic nitrate, and ammonium, in the soil solution.

There are two opposing biological processes in principle which continuously interchange between the organic and inorganic nitrogen forms in the soil. Soil microorganisms decompose organic materials to yield inorganic materials as byproducts. Soil microflora utilize inorganic materials to synthesize new organic tissues. The conversion of organic to inorganic is referred to as mineralization and the conversion of inorganic to organic as immobilization. The magnitude of each process for a given time interval depends on many factors, including the nature of organic material and the gross size and activity of the soil microflora during the time interval. In describing these processes in terms of a gross model, kinetic approach appears appropriate because the reaction times involved in microbial nitrogen transformations are of the order of several days or weeks.

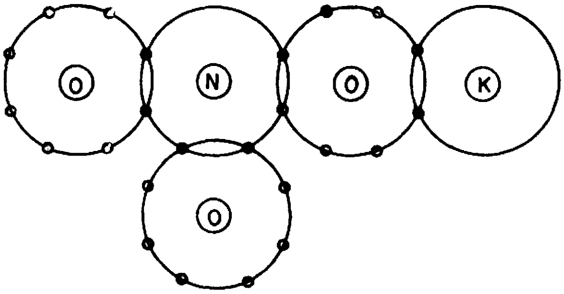
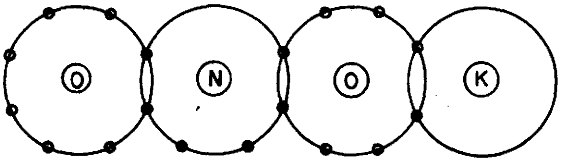
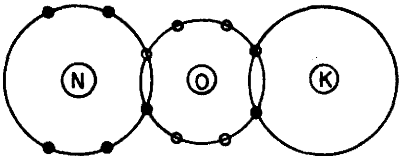
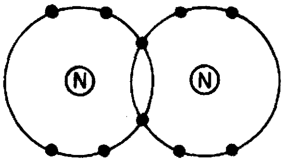
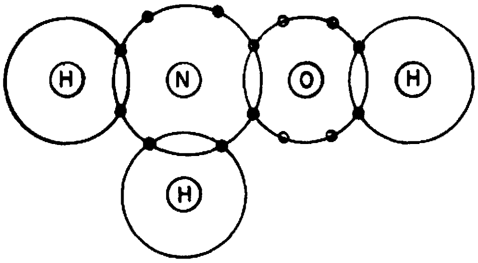
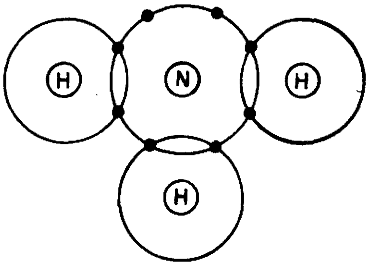
Valence	Compound	Formula	Valence Electrons
+5	**Nitrate Ion**	NO_3^-	
+3	**Nitrite Ion**	NO_2^-	
+1	**Nitroxyl**	[HNO]	
0	Nitrogen Gas	N_2	
- 1	Hydroxyl-amine	$HONH_2$	
- 3	Ammonia	NH_3	

Figure 11. Number of oxidation levels of nitrogen in soil profile. (After Delwiche, 1970)

Model development

In developing the transformation model the following discussion outlines the techniques adopted from Dutt et al. (1972). Described by Figure 8 is a conceptual model of the biological transformations of nitrogen within a soil profile. The inputs and outputs of the system model are illustrated in Figure 12, and the basic pathways of transformation conceived in the conceptual model are quantified by considering the following rate equations.

1. Hydrolysis of Urea.
2. Mineralization and immobilization of ammonium-nitrogen and organic nitrogen.
3. Nitrification of ammonium-nitrogen.
4. Immobilization of nitrate-nitrogen.

Mathematical equations for the transformation pathways described above have been developed from experimental data published by several authors and shown by Table 2. These equations are arrived at by computer oriented statistical analysis, namely least squares multiple regression analysis.

For modeling purposes the basic equation of transformation of a nitrogeneous species can be represented by the following equation:

$$R = f[\mathrm{TUREA}, \mathrm{TNH_3}, \mathrm{AOR}, \mathrm{TNO_3}, \mathrm{TEMP}, \mathrm{TEN}, \mathrm{CNR}]. \qquad (4.1)$$

in which

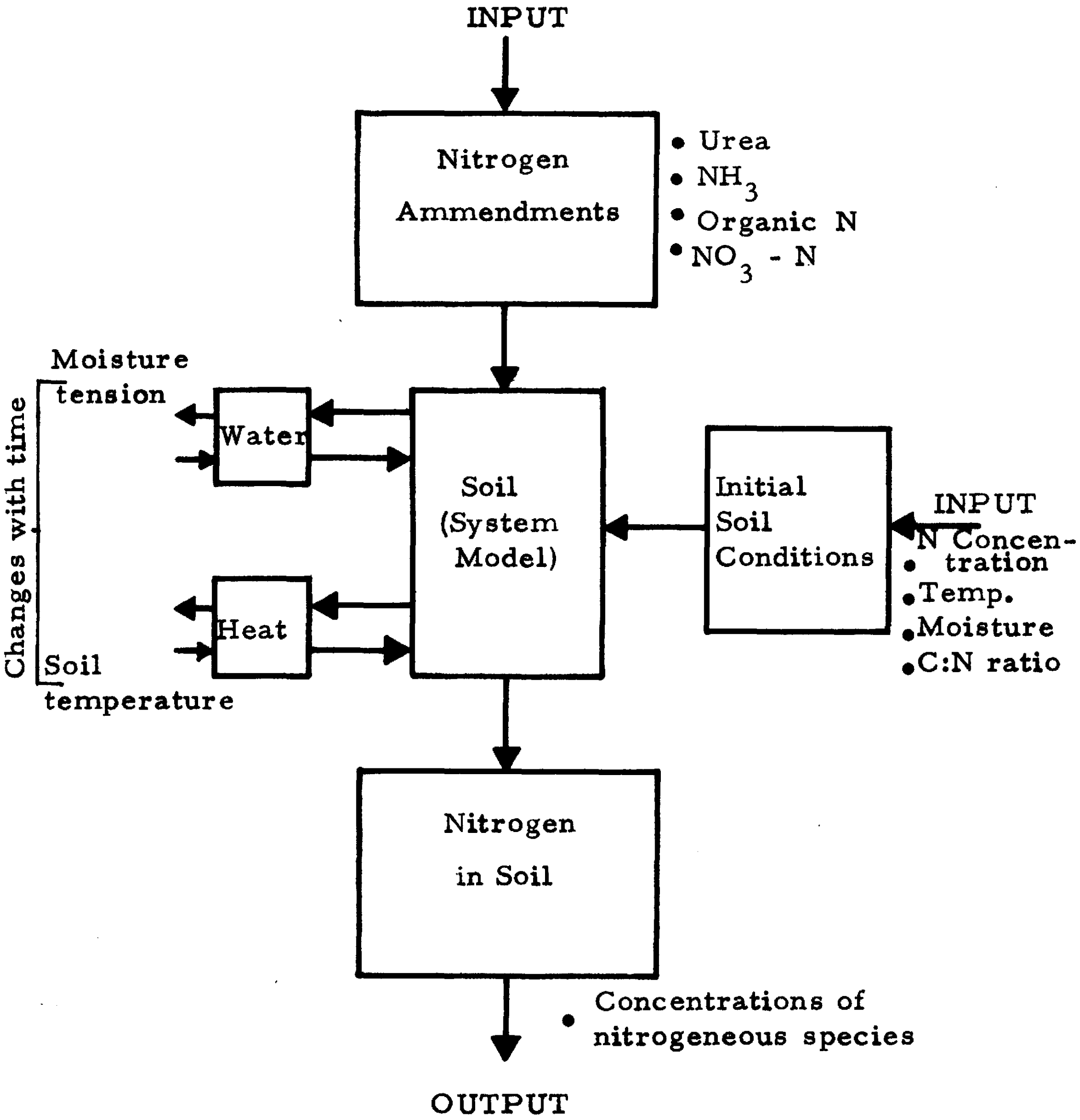


Figure 12. Basic inputs and outputs of the nitrogen transformation model.

R = rate of transformation of N-species (unit/time)

TUREA = concentration of Urea-N

TNH_3 = concentration of NH_4^+

AOR = concentration of organic-N

TNO_3 = concentration of NO_3^--N

TEMP = soil temperature

TEN = soil moisture tension

CNR = carbon: nitrogen ratio of organic matter

Table 2. Source of experimental data adopted for transformation pathways of nitrogen.

N	Transformation Pathway	Source of experimental data
1.	Hydrolysis of Urea	Broadbent, Hill, and Tyler (1957) Overrein and Moe (1967)
2.	Mineralization and immobilization	Broadbent (1957, 1966) Alexander (1961)
2a.	Correction for C:N ratio	Alexander (1961), Broadbent (1957)
3.	Nitrification	Broadbent, Tyler, and Hill (1957a) Justice and Smith (1962)
4.	Nitrate immobilization	Broadbent (1966)

Using multiple linear regression technique, the general form of the rate equation (4.1) could be more explicitly written as:

$$R = c + b_1 x_1 + b_2 x_2 + \ldots + b_n x_n \quad . \quad . \quad . \quad . \quad . \quad (4.2)$$

in which

R = rate (dependent variable)

c = a constant (Y - intercept)

x_n = an independent variable

b_n = a constant (regression coefficient)

Various combinations of independent variables were tried to obtain the best fit as evidenced by the multiple correlation coefficient and F-ratio. Only those variables or variable combinations making significant contributions to the regressions were included in the final equations. Interdependence of the independent variables, however, was not considered in developing the rate equations. The regression equations are valid even though there is interdependence of some of the independent variables.

Development of rate equations

1. Urea hydrolysis rate equation. The basic variables considered in the development of the urea equation were the temperature (^{o}C) and the concentration of urea-N (microgram/gm of soil). The independent variables in the final equation were $\log_{10}$ temperature (^{o}C) and $\log_{10}$ urea-N concentration, which gave best fit results.
2. Mineralization and immobilization rate equation. A single equation was derived for the net rate of NH_4^+ - N immobilization or the net rate of organic - N mineralization depending on the sign. A negative rate indicates loss of

organic residue (mineralization). A positive rate shows a sign of gain of microbial cell material (immobilization).

The basic parameters used in this equation are the temperature (^{o}C), the concentration of organic-nitrogen (micrograms/gm of soil), the NH_4^+ - N concentration (microgram/gm of soil), and the C:N ratio of the organic residue. The final equation contains the temperature, the organic - N concentration, and the $\log_{10}$ NH_4^+ - N concentration as the independent variables.

3. <u>Nitrification rate equation.</u> The nitrification rate equation represents the net transformation of NH_4^+ - N to NO_3^- - N . This means that conversion of some NO_3^- - N to NH_4^+ - N is allowed in the model. However, the net result always is assumed to be the appearance of NO_3^- - N . The basic variables used to develop the equation were the temperature (^{o}C), and the concentration of NH_4^+ - N (ug/g soil), the concentration of NO_3^- - N (ug/g soil, and the soil moisture tension (bars). The independent variables included in the final equation, however, are temperature times the NH_4^+ - N concentration, the $\log_{10}$ NH_4^+ - N concentration, and the $\log_{10}$ NO_3^- - N concentration.

4. <u>NO_3^- - N immobilization rate equation.</u> The NO_3^- - N immobilization equation quantifies the conversion of

NO_3^- - N to microbial cell material. As in the case of NH_4^+ - N immobilization, the process is assumed to take place only at C:N ratios greater than 23. The equation does not allow direct NO_3^- - N formation from organic-N, since this transformation pathway is highly unlikely. The basic variables used to develop the final equation were the following:

$$\frac{\text{temperature } (^{o}\text{C})}{(\text{organic-N concentration})^2 \atop (\text{ug/g soil})}\ ,\ e^{(\text{temperature})}$$

and

$$\frac{\text{temp. x (organic-N - } NO_3^- \text{ - N concentration)}}{\text{organic - N concentration}}$$

Tables 3 and 4 describe in detail the various transformation equations developed by Shaffer et al. (1969). Shown in these tables are also the correlation coefficients indicating the goodness of fit of these equations with the experimental data referenced in Table 2. Actual model development necessitated certain corrections in the coefficients of the equations to provide a better fit with observed data. Represented in Table 5 is a summary of corrections made in the regression coefficients.

The rate equations so developed have limitations with regard to the ranges of temperature, soil moisture

Table 3. Variables, constants, and statistical tests for the urea hydrolysis and mineralization-immobilization rate equations. (After Shaffer et al., 1969.)

Equation	Urea Hydrolysis	Mineralization-Immobilization
Variable:	$\log_{10}T$	T
r Value:*	$6.22\cdot10^{-1}$	$-5.85\cdot10^{-1}$
Coefficient (b1):	$-1.56\cdot10^{2}$	$-2.16\cdot10^{-3}$
Variable:	$\log_{10}$ urea-N	organic-N
r Value:	$6.78\cdot10^{-1}$	$-7.69\cdot10^{-1}$
Coefficient (b2):	$-1.53\cdot10^{2}$	$-2.70\cdot10^{-2}$
Variable:	—	$\log_{10}$ ammonia-N
r Value:	—	$7.06\cdot10^{-1}$
Coefficient (b3):	—	$3.92\cdot10^{-1}$
Constant:	$4.13\cdot10^{2}$	$8.92\cdot10^{-1}$
F Ratio:	$6.24\cdot10^{1}$	$3.89\cdot10^{1}$
R^2 Value:**	$7.23\cdot10^{-1}$	$7.40\cdot10^{-1}$
SEE:***	$4.90\cdot10^{1}$	$2.45\cdot10^{-1}$

* Simple Correlation Coefficient
** Multiple Correlation Coefficient Squared
*** Standard Error of Estimate for the Rate

Table 4. Variables, constants, and statistical tests for the nitrification and nitrate-N immobilization rate equations. (After Shaffer et al., 1969.)

Equation	Nitrification	Nitrate-N Immobilization
Variable:	T x (ammonia-N)	T/(organic-N)^{2}
r Value:	$5.44 \cdot 10^{-1}$	$4.18 \cdot 10^{-1}$
Coefficient (b1):	$1.62 \cdot 10^{-3}$	$1.52 \cdot 10^{0}$
Variable:	log$_{10}$ ammonia-N	e^{T}
r Value:	$3.61 \cdot 10^{-1}$	$-2.82 \cdot 10^{-1}$
Coefficient (b2):	$2.38 \cdot 10^{-1}$	$-3.23 \cdot 10^{-15}$
Variable:	log$_{10}$ nitrate-N	(T x (organic-N)-(nitrate-N))/(organic-N)
r Value:	$-4.97 \cdot 10^{-1}$	$3.24 \cdot 10^{-1}$
Coefficient (b3):	$-2.51 \cdot 10^{0}$	$-4.90 \cdot 10^{-3}$
Constant:	$4.64 \cdot 10^{0}$	0.0
F Ratio:	$2.91 \cdot 10^{1}$	$9.96 \cdot 10^{0}$
R^2 Value:	$3.84 \cdot 10^{-1}$	$4.21 \cdot 10^{-1}$
SEE:	$3.67 \cdot 10^{0}$	$4.11 \cdot 10^{-1}$

Table 5. Summary of corrections made in regression coefficients. (After Shaffer et al., 1969.)

Equation	C:N Ratio	b1	b2	b3
Urea Hydrolysis	—	NC*	NC	—
Mineralization-Immobilization	< 23	NC	NC	$1.60 \cdot 10^{0}$
	≥ 23	NC	NC	$7.83 \cdot 10^{-1}$
Nitrification	<23	NC	$4.50 \cdot 10^{0}$	NC
	≥23	$8.00 \cdot 10^{-4}$	$2.38 \cdot 10^{-4}$	$-2.10 \cdot 10^{0}$
Nitrate-N Immobilization	< 23	NC	NC	NC
	≥23	NC	NC	NC

* NC = No Change.

tension, and C:N ratio. The computed rate of a transformation pathway is, therefore, corrected for each of the above factors, as detailed below.

5. Correction for C:N ratio. The rate equation was derived for an available data corresponding to a C:N ratio of 80. The correction factor is derived using a linear equation involving C:N ratio. The final equation form is as follows:

$$M = -2.51 + 1.85 \times \log_{10} (\text{C:N ratio}) \quad . \quad . \quad (4.3)$$

in which

M = correction factor, which is unity at C:N ratio of 80 and zero at C:N ratio of 23

It is assumed that the net immobilization occurs above C:N ratio of 23. The net rate at 23 is assumed to equal zero.

6. Low temperature correction. Exponential rate functions were used to adjust the output of the regression rate equations for temperatures less than 10°C, and the rates become equal to zero at about 4°C. The original rates were, therefore, multiplied by the output from a logarithmic function based on the temperature. No upper limits or corrections were necessary for higher temperatures because the equations appeared valid at most

maximum soil temperatures occurring below the surface.

7. Moisture correction. Exponential moisture functions were used to correct the regression equations for tensions below about 10 bars. No correction was, however, applied to Urea hydrolysis equation, as there was no evidence to suggest a moisture correction in the moisture range considered in this study. It is assumed that the rate equation is valid at field capacity (1/3 bar).

8. Prediction of C:N ratio in soil profile with time. Since the C:N ratios of organic residues change as decomposition progresses, a method was developed to predict the C:N ratios with time. Alexander (1961), and Buckman and Brady (1960) have shown that microorganisms release about 30 carbon atoms from organic residues for every nitrogen atom consumed. The N may come from the organic residue or from NH_4^+ in the soil water or on the exchange complex. The C either is released as CO_2 or used to produce microbial cell material. The N may be transformed to NH_4^+ or used in the production of cell material.

The initial amount of C in the organic residue is estimated by multiplying the amount of residue by 0.4. Likewise, the initial amount of N in the residue is approximated by multiplying the amount of residue by 0.4/C:N ratio. If the ratio is greater than 23, the amount of residue carbon remaining after some time interval is approximated by subtracting 30 times the predicted amount of organic-N immobilized from the amount of residue C present at the start of the interval. The amount of residue N is assumed to remain constant. That is, it is assumed that the microorganisms consume only the NH_4^+ mineral form of N in this C:N ratio range. The new C:N ratio is computed by dividing the amount of residue C by the amount of residue N.

At C:N ratios less than or equal to 23, the residual amount of C is computed in the same manner except that the amount of N mineralized is used as the computation base. The new amount of residue N is determined by subtracting the amount of N mineralized during the time interval. In this case the assumption is made that the microrganisms derive N only from the organic residues in this C:N ratio range. Again, the ratio is computed by dividing the amount of residue C by the amount of residue N.

When the amount of organic residue becomes equal to zero, the ratio is set equal to the average C:N ratio for the soil (e.g., in the range 5-15). This allows for mineralization of dead microbial cells with time.

Temperature estimates in the root zone of the soil profile

Temperature variation at the top of soil profile has marked effect on the fluctuation of temperature in the subsoil. It depends on many factors, including soil-water content, the apparent thermal diffusivity of the soil, and the depth below the soil surface. Prediction of the temperature variation with depth is, therefore, quite complex. Numerical procedures using digital computers is one of the easier and reliable methods to solving this problem.

Wierenga and DeWit (1970) have developed a mathematical model to simulate heat transfer through soils. In the present study, however, no separate mathematical model is incorporated for temperature simulation within the soil profile on account of the following reasons:

1. The maximum range of fluctuation in temperature is nearer the top soil. There is an averaging effect caused by assuming the biological transformations to occur within the root zone and also in assuming that these transformations are occurring in the topmost soil layer. This averaging effect will smooth the temperature fluctuations.
2. The overall system model is already too complicated and addition of a temperature simulation model would call for a higher degree of sophistication not intended in the system model.

3. The model has a monthly time increment with optional spatial resolution which will further dampen the fluctuation in temperature. A reasonable estimate is therefore made with regard to the average temperature in the root zone of the soil profile, within the time increment of the model.

Sign convention and rate units

In all the basic rate equations a positive sign indicated a gain and a negative sign a loss with respect to that particular constituent. The rate units for all the rate equations used in this transformation model were expressed in ppm/day.

Method of solving the rate equations

Since the rate equations predicted the changes in concentrations of nitrogeneous species in ppm/day, the problem was one of computing these changes in terms of the time increment of one month for the overall system model. This problem was resolved with the following considerations:

1. Fertilizer applications and organic matter turn over to soil were assumed to have a spatial uniformity over the entire study area. Local variations were ignored.
2. Since the developed model was general in nature with the object of predicting the concentrations of ions in the return flows, no special consideration was given to the

vertical distribution of concentrations of NO_3^- within the zone of root influence.

3. The majority of biological transformations were assumed to occur within the root zone. Their effect below the root zone was, therefore, neglected.
4. Time increments in the order of fractions of a day in predicting the transformations of nitrogeneous species, as adapted in the dynamic model by Dutt et al. (1972), could give the model a much higher degree of sophistication and could involve in utilizing excessive computer time. This was not worth the trouble in terms of the objectives of this gross model.

In view of the above considerations, the non-linear system was, for modeling purposes, linearized even beyond the stage of regression analysis of the experimental data. It was assumed that the predicted values of transformations of nitrogeneous species in ppm/day were uniform within the time increment of the overall model. The net rate of each transformation was, therefore, multiplied by the days in a month.

Abstractions of nitrogen from the system

The quantity of nitrogen in the soil water system is to be accounted for loss and use processes, as shown in Figure 13 (Bartholomew, 1972). Losses due to denitrification are assumed to be

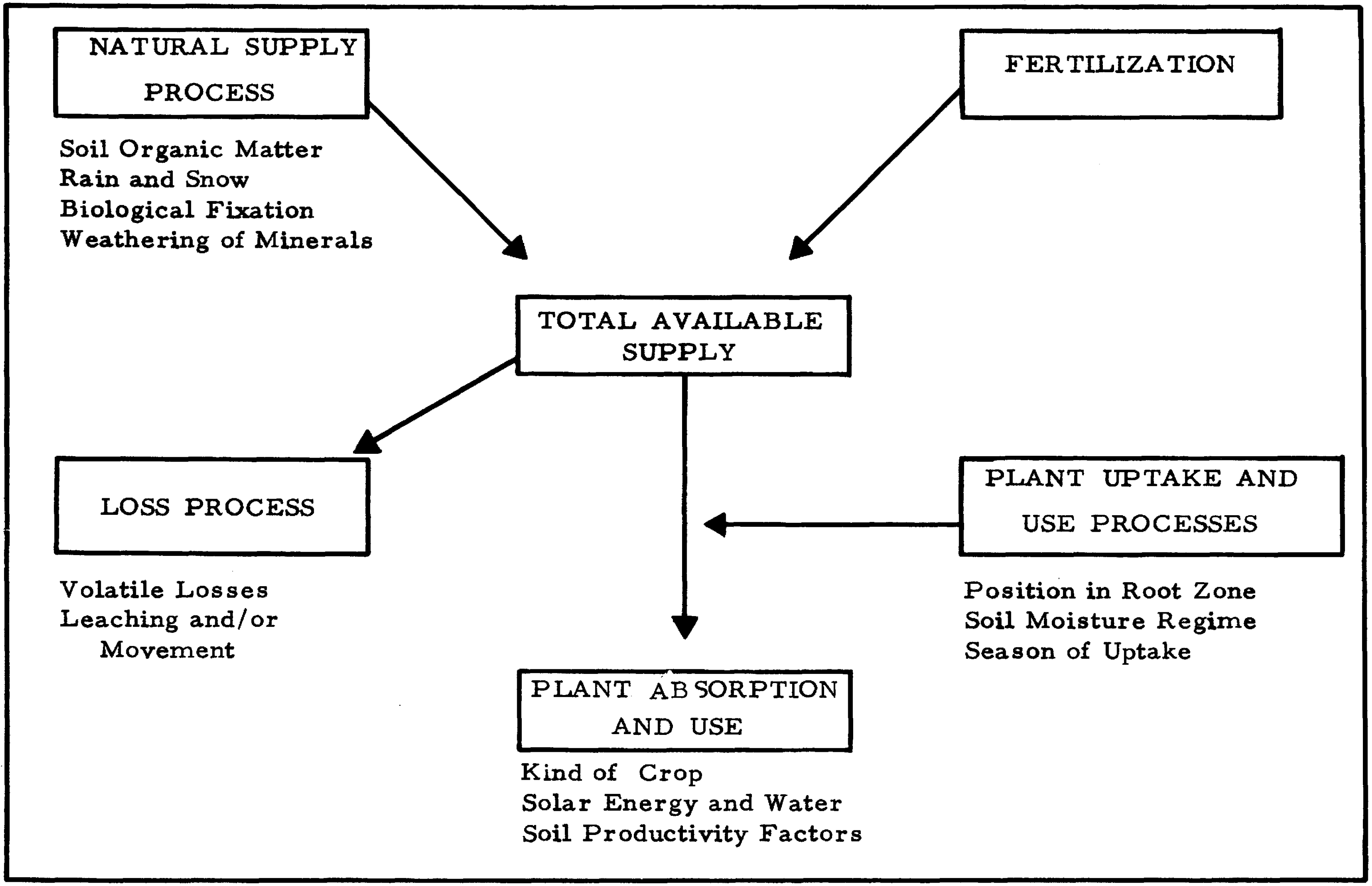


Figure 13. A perspective view of soil nitrogen supply, loss, and use processes. (After Bartholemew, 1972).

negligible as the system is generally considered aerobic within the soil profile. The losses due to leaching of $NO_3^- - N$ to the ground water is of interest in this study. The use processes consist of crop uptake of nitrogen from the soil water system and also for the uptake of nitrogen by the growing aquatic biomass in the overland flow. Quantifying these use processes involves identification of many parameters for both the processes as discussed below.

Crop uptake of nitrogen. Nitrate and ammonium ions are the primary forms in solution that are used by growing crops. The quantity of uptake depends on many factors, including the quantity of available nitrogen in soil solution, growth stage of crop, moisture content of the soil, kind of nitrogen carrier and climatic region. The methods for assessing the uptake of nitrogen by crops considered in this study are the following.

1. To assume that the uptake is directly proportional to the root density in the soil profile. This requires extensive data on the variation in root distribution with increase in depth of the soil. It differs mostly from crop to crop and also with the growth stage of crops.
2. To assume that the uptake is proportional to the consumptive use of water. In this case, a proportionality constant is to be arrived at based on previous experiments, sound engineering judgment, or by model calibration.

3. To have a data on the average distribution of uptake of nitrogen with time. This requires practical tests on the nitrogen content of each crop at each stage. In arriving at these figures, an assumption is made that the plant root distribution is independent of time.

In this study the monthly uptake values are estimated on the lines indicated by the last method as above. The estimated values have similar trends presented by Dutt et al. (1972), and compare favorably with the assessed annual quantities of uptake.

Nitrogen uptake by aquatic biomass. Loss of nitrogen in the overland portion usually occurs by way of utilization by the growing aquatic biomass, namely, algae and vegetation. The quantity of uptake depends on many factors, including temperature, contact time, amount of N available to the growing biomass, and the quantity of biomass itself. Establishing this quantity of uptake is beyond the scope of this study, as it involves collection of additional experimental data. This can be a separate research by itself. However, a correction factor is introduced in the model to represent the loss of nitrogen in the overland flow of the return flow as shown in the following equation:

$$Q_{net} = Qi \quad *UBIOM\ (I) \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (4.4)$$

in which

I = time increment

Q_{net} = net quantity of nitrate in the return flow

Qi = species (nitrate) concentration in the subsurface water contributing to surface runoff as computed by Equation (3.11)

UBIOM = fraction of N after uptake by aquatic biomass (less than or equal to one). This is correlated with the average temperature of water.

All the quantities on the right hand side of Equation (4.4) having been identified, the modeling procedure involved in solving the equation for Q_{net}, the net quantity of nitrate in the return flow.

CHAPTER V

THE COMPUTER PROGRAMS OF THE SYSTEM

Introduction

The overall model of the system consists of three individual submodels. These are the hydrologic, chemical and biological transformation models. While the hydrologic portion of the program is written specifically for the Snake River basin at Twin Falls, Idaho, the chemical and biological programs are general in nature. With minor changes, the entire model could be applied to other areas as well.

The hydrologic portion of the program utilized a hybrid computer, while the chemical and biological programs operate on digital computer. The EAI 580 Analog/Hybrid computing system and the EAI 640 Digital computing system are utilized for the hydrologic, chemical and biological models, respectively. The program was written in FORTRAN IV.

The computer models for chemical reactions and biological transformations are similar to those developed by Dutt et al. (1972). The hydrologic portion of the model, however, is a combination of the models developed by Thomas et al. (1971) and Hill et al. (1973). A complete listing of the entire program and definition of variables are shown by Appendices B and C. A detailed description of the computer programs developed for the overall system envisioned in this study is presented in this chapter.

The Computer Model

The combined system model consists of a main program and twentyone subprograms. The subprograms are designated as: (1) HYDSM, (2) BASIC, (3) HYDDAT, (4) PRETEM, (5) POTST, (6) PARSET, (7) GRAPH, (8) QUAL, (9) CONINP, (10) EQEXCH, (11) SOIL, (12) AVQLTY, (13) XCHNGE, (14) SALT, (15) ANDAT, (16) UPTAKE, (17) TRNSFM, (18) RATE 1, (19) RATE 2, (20) RATE 3, (21) RATE 4.

Subprograms 1 through 7 pertain to the hydrologic portion of the model. The chemical quality portion utilizes subprograms (8) through (14), while the biological portion contains the subprograms (15) through (21). A generalized flow chart for the overall program is represented by Figure 14.

MAIN program

The main program is the driving program for the entire simulation model. Figure 15 represents the general flow chart of the main program. This program is similar to the techniques developed by Hill et al. (1973). Major operations of the main program, listed in the order of performance, include the following to suit the overall system simulation.

1. Control the operation of analog computer through the hybrid linkage routines QSHYIN, QSC, QSSECN, and QSDLY.

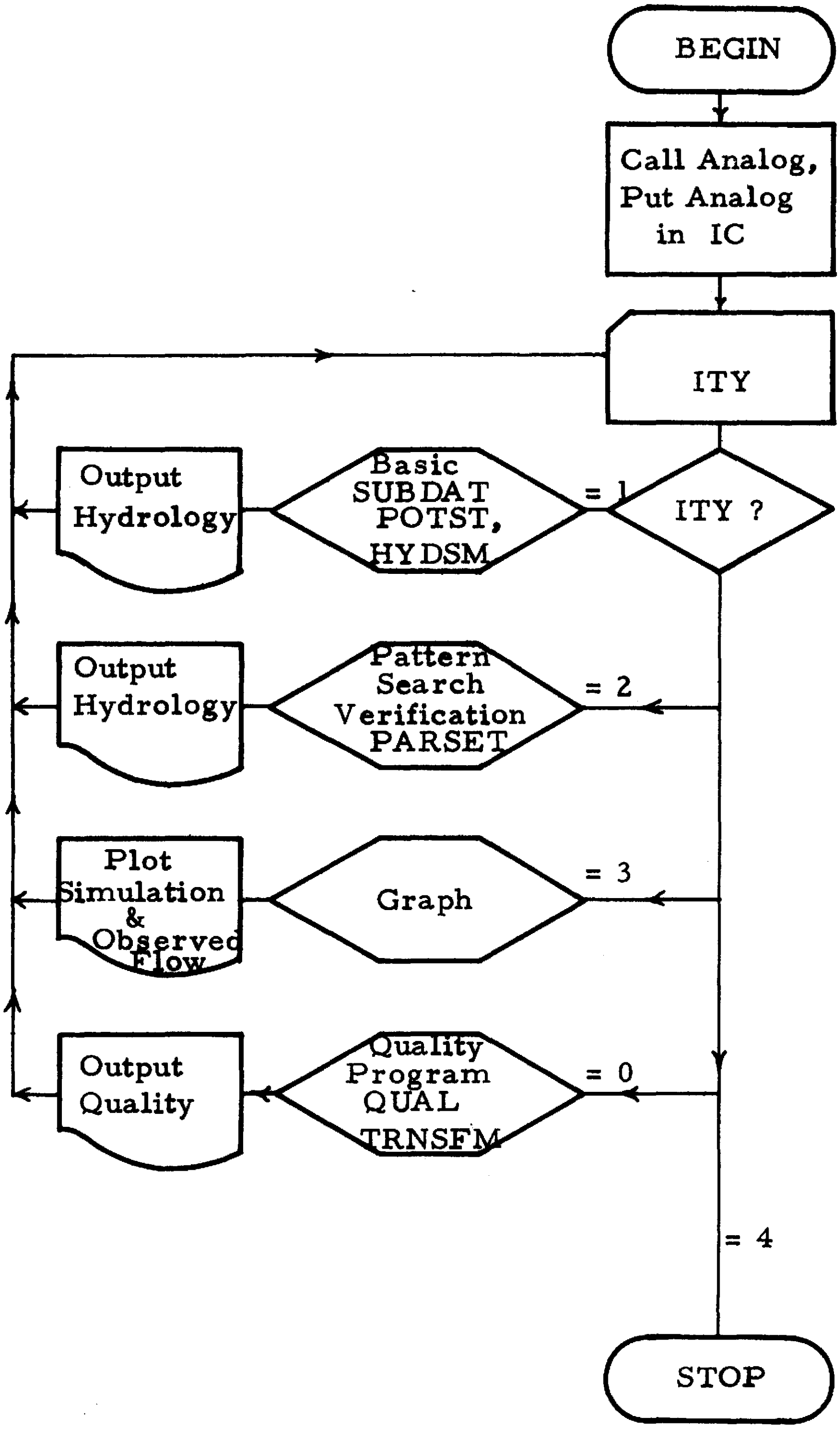


Figure 14. Generalized flow chart of overall program.

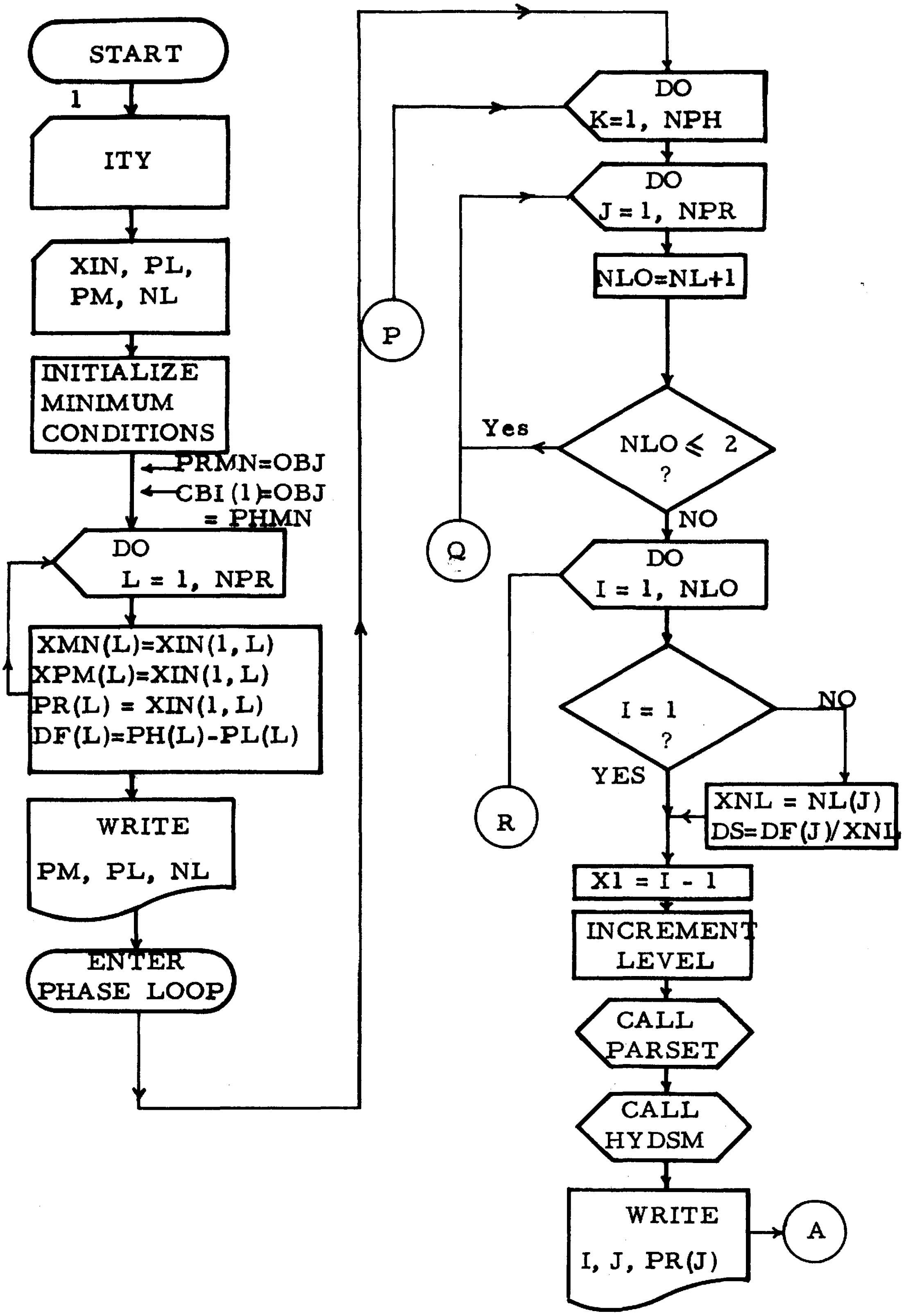


Figure 15A. Generalized flow chart of MAIN.

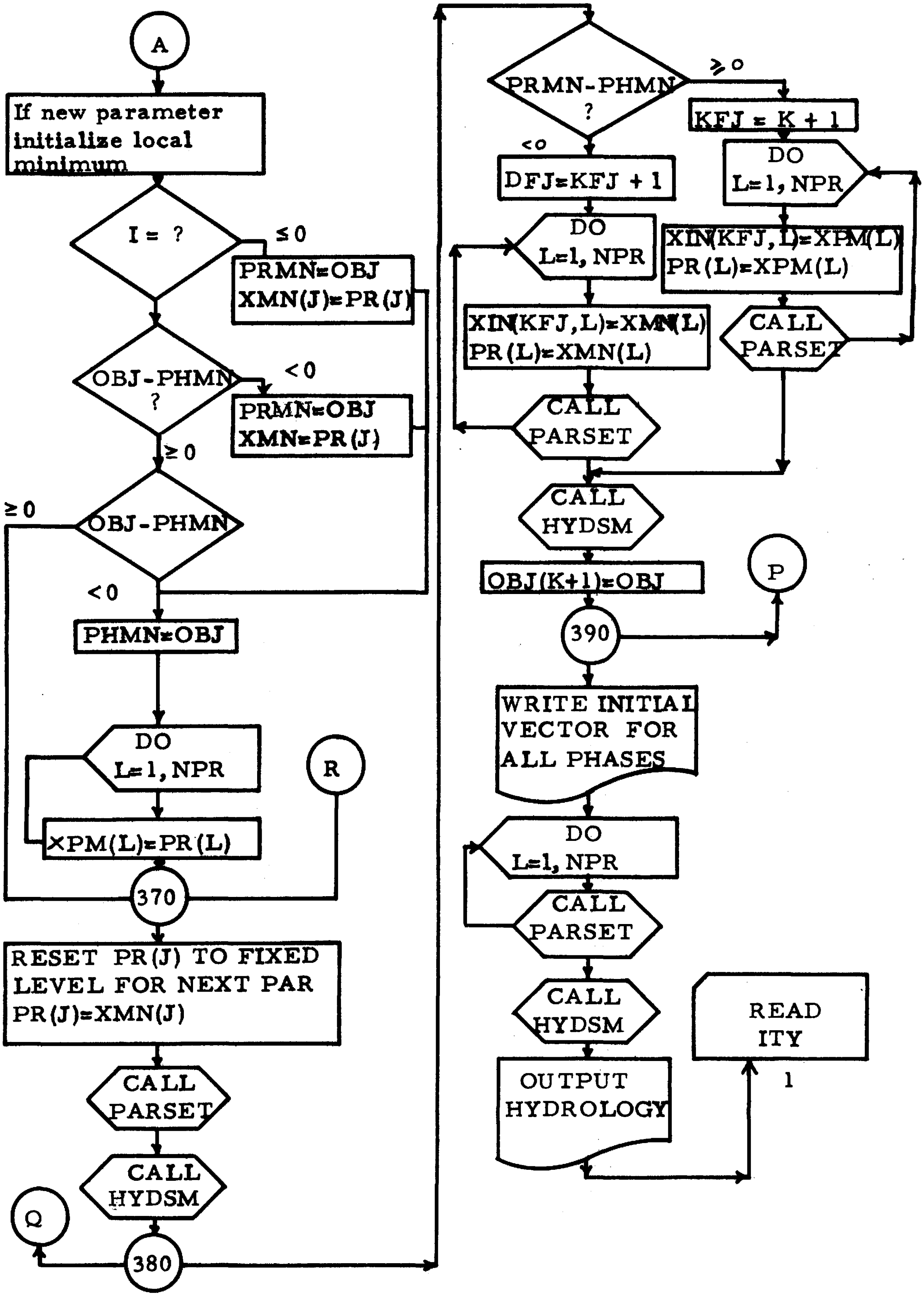


Figure 15B. Generalized flow chart of MAIN.

2. Simulate the output from the system hydrology through the subroutine HYDSM and compute the objective function. (Data is, however, assembled by HYDSM through the subroutines BASIC, HYDDAT, and PRETEM, while the potentiometers in the analog are set through subroutine POTST.) The objective function adopted in this study is sum squares of differences between computed and observed outflows.
3. Perform optimization of various parameters to minimize the objective function through statement 80. (Pattern search technique outlined by Hill et al. (1973) is adopted in this program.) Each time the potentiometer values in analog computer are set through subroutine PARSET.
4. Operate HYDSM with the optimum parameters and plot (optionally) the outflow hydrograph, both the observed and computed, through the subroutine GRAPH.
5. Chemical quality subprogram, QUAL, is called to predict the chemical quality of outflow.

The input data list for the main program is shown in Appendix D.

Hydrologic model

The hydrologic model is programmed on a hybrid computer and is described by the subroutine HYDSM. The general flow chart for the basic hydrologic model is adopted from Figure 5 to suit the study area. The wiring diagram of the analog portion of the hydrologic model is shown in Figure 16. The operation of HYDSM, in sequential order, is as follows:

1. To compute the value of various hydrologic relationships described in Chapter III in terms of the particular area being modeled.
2. To control the analog computer timing and operation.
3. To predict the monthly quantity of outflow and compare it with observed value.
4. To store the values of various quality parameters required by the subprogram QUAL.

The program starts with assembling initial crop and hydrologic data through the subroutines BASIC and SUBDAT. Then the quantities of snowmelt, precipitation and evapotranspiration (using modified Blaney-Criddle method) are computed in the subroutine HYDSM. These values are transferred as inputs to analog portion. Values of component parts of the right hand side of Equation (3. 3) are computed in the analog portion and transferred back to digital portion of HYDSM to compute total surface runoff, (SUMOUT), during the month. The process is repeated for all months and all years.

The analog portion of the hybrid simulation is a combination of portions described by Hill et al. (1973) and Thomas et al. (1971) to suit the study area, and to facilitate usage of analog portion more

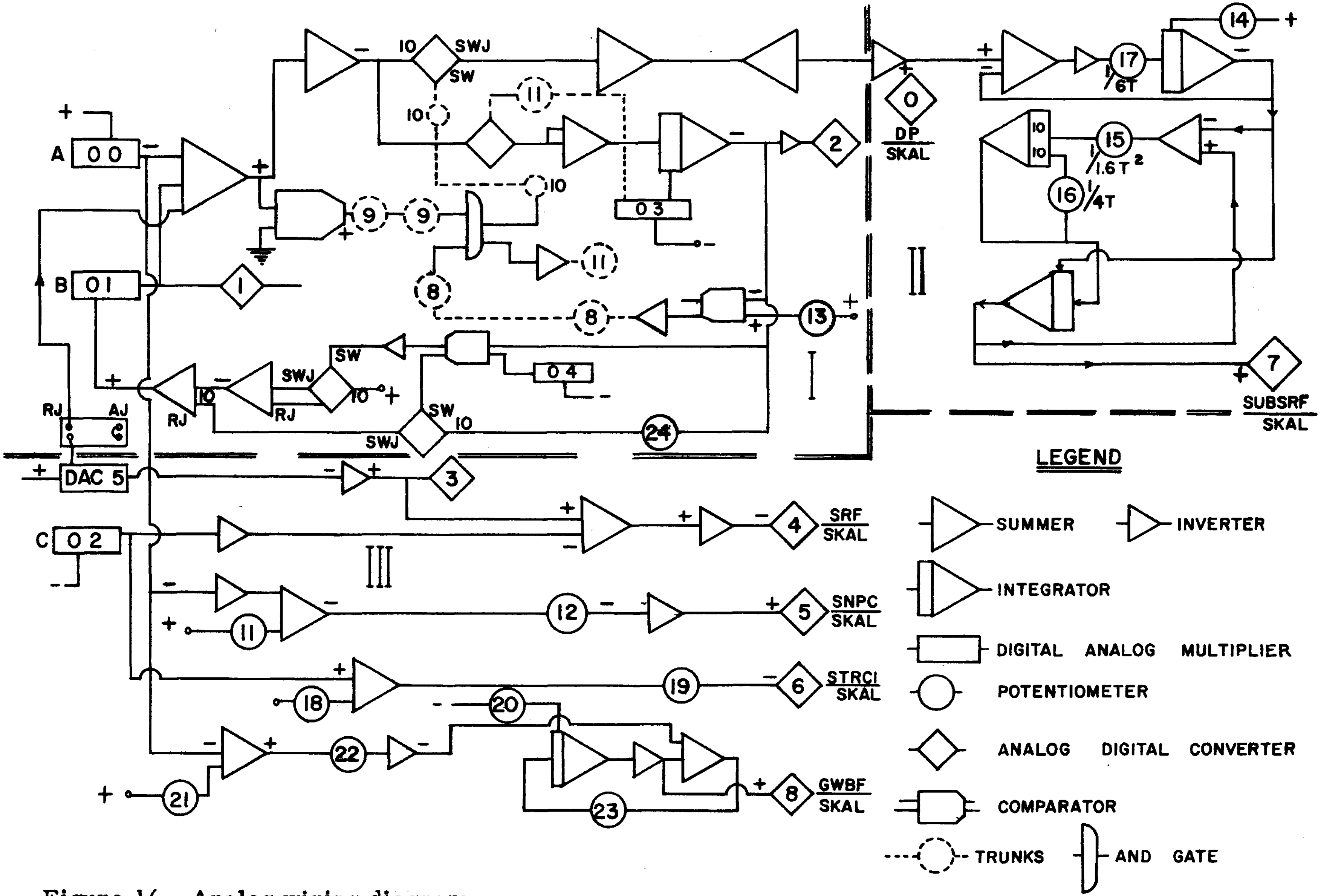


Figure 16. Analog wiring diagram.

efficiently. The analog portion performs essentially three major functions: (1) it keeps an account of soil moisture; (2) it integrates and routes the deep percolation to simulate the subsurface outflow; and (3) it routes the inflow groundwater and performs some miscellaneous calculations that could be done equally well on either the analog or the digital, but which are better performed on the analog during verification. These three important functions are executed in the areas designated I, II, and III, respectively, on the wiring diagram (Figure 16). The areas I and II are discussed in detail by Hill et al. (1971, 1973), while the area III is discussed by Thomas et al. (1971).

The input data list for the subroutines BASIC and HYDDAT utilized by the subprogram HYDSM are shown in Appendix D.

Details of quality simulation program (subroutine QUAL)

After the observed and computed outflows are optionally plotted in the hydrologic portion of the simulation program, the control calls the quality program, QUAL. Hydrologic quantities needed to be used in the quality program as input values are preserved in the common storage of the computer. Shown in Table 6 is the list of parameters required by QUAL as input from HYDSM. This list, incidentally, describes the various quantities from the hydrologic subsystem that are required as inputs to QUAL for an all digital program. Observed values of average monthly concentrations of individual ions in the surface outflows are computed separately to economize in the run-time of computers.

Table 6. Parameters in common from HYDSM to QUAL.

Mnemonic	Description
SRF_I	Overland portion of total runoff in month I.
SUBSRF	Sub surface component of total runoff
GWBF	Routed ground water inflow
SNPC	Ungaged runoff correlated to precipitation and snow melt
DAL	Quantity of water applied to land
$STRC_1$	Ungaged surface runoff correlated to canal diversion
DP	Deep percolation
SUMOUT	Computed quantity of total runoff
SMCH	Change in soil moisture of root zone in time I
SM	Average moisture content of root zone

These are read in first through subroutines CONINP, UPTAKE, ANDAT, and SOIL. Details of data read in by these subroutines is shown in Appendix D. Figure 17 shows the flow chart of the subroutine QUAL. The program proceeds into a Do loop to statement 3000 for each kind of soil modeled in the study area. The equilibrium

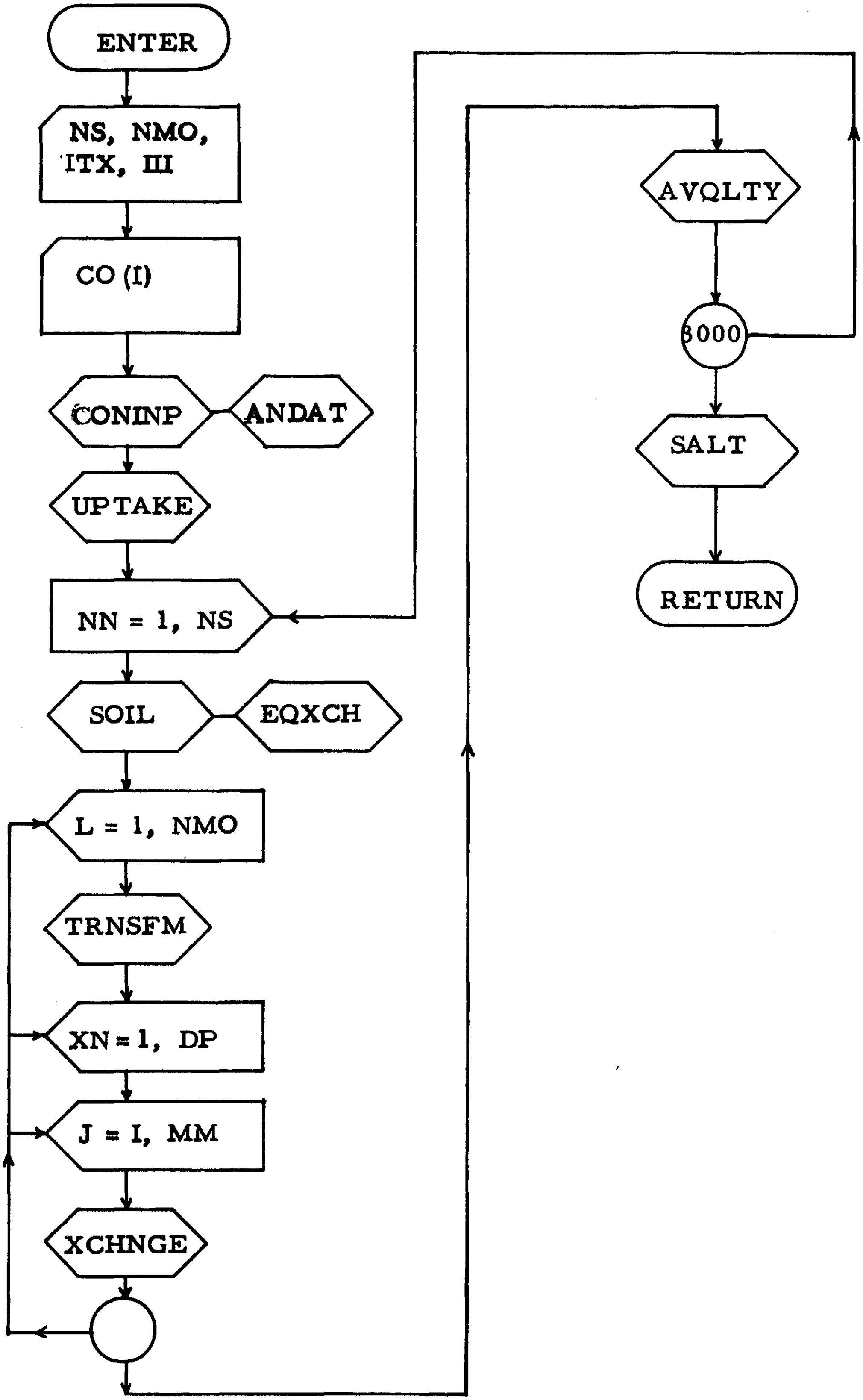


Figure 17. Generalized flow chart of subroutine QUAL.

concentrations of ions in the initial soil solution are computed through the subroutines EQEXCH (from subroutine SOIL) for the first time based on the initial soil analysis. Then the program consists in simulating the percolation of the applied water to the land (DP) each month in a piston flow type of displacement vertically downward through the assumed number of layers of the type of soil under consideration.

At this stage of the program the subroutine TRNSFM is called to predict the nitrogen transformations in the root zone (the topmost soil layer). The computed values of nitrate and ammonium ions are then corrected for crop uptake of these ions. An assumption is made here that the available quantity of nitrogen is the limiting value for crop uptake. The resultant quantity of nitrogen after crop uptake is, therefore, adjusted to zero for all negative values. The concentration of nitrate-N is then utilized for all equilibrium calculations of soil solution for purposes of computing increased ionic strength in the subroutine XCHNGE. Ammonium is not considered in adding to the ionic strength of soil solution as its concentration is usually insignificant in value.

In each soil layer an equilibrium concentration is assumed to be attained in respect to every ion. These equilibrium calculations are performed in an iterative procedure through the subroutine XCHNGE. For each layer the various equilibrium and exchange reactions considered in the program are listed in Figure 7.

The average concentration of each of the ions in the subsurface return flow is computed next through the subroutine AVQLTY. The total quantity of salt outflow is then computed in the subroutine SALT by multiplying the respective ionic concentrations with the corresponding simulated quantities of outflow from the hydrologic portion of the program, the HYDSM. The concentration of NO_3^- is, however, corrected for uptake of NO_3^- by aquatic biomass.

Biological transformation model (subroutine TRNSFM)

A generalized block diagram of subroutine TRNSFM developed by Dutt et al. (1972) is shown in Figure 18a. However, modifications in the program developed by Dutt et al. (1972) were found necessary to suit the gross nature and large time increments of this model. Figure 18b represents the block diagram of TRNSFM followed in the study and Figure 19 represents the corresponding flow chart of this subroutine.

Construction and operation

The following discussion is adopted from Dutt et al. (1972) to describe the construction and operation of TRNSFM developed in this study.

The subroutine consists of Urea-N, organic-N-C:N ratio, NH_4^+ - N, and NO_3^- - N sections. These sections are independent of each other so far as sequence is concerned. That is, the order

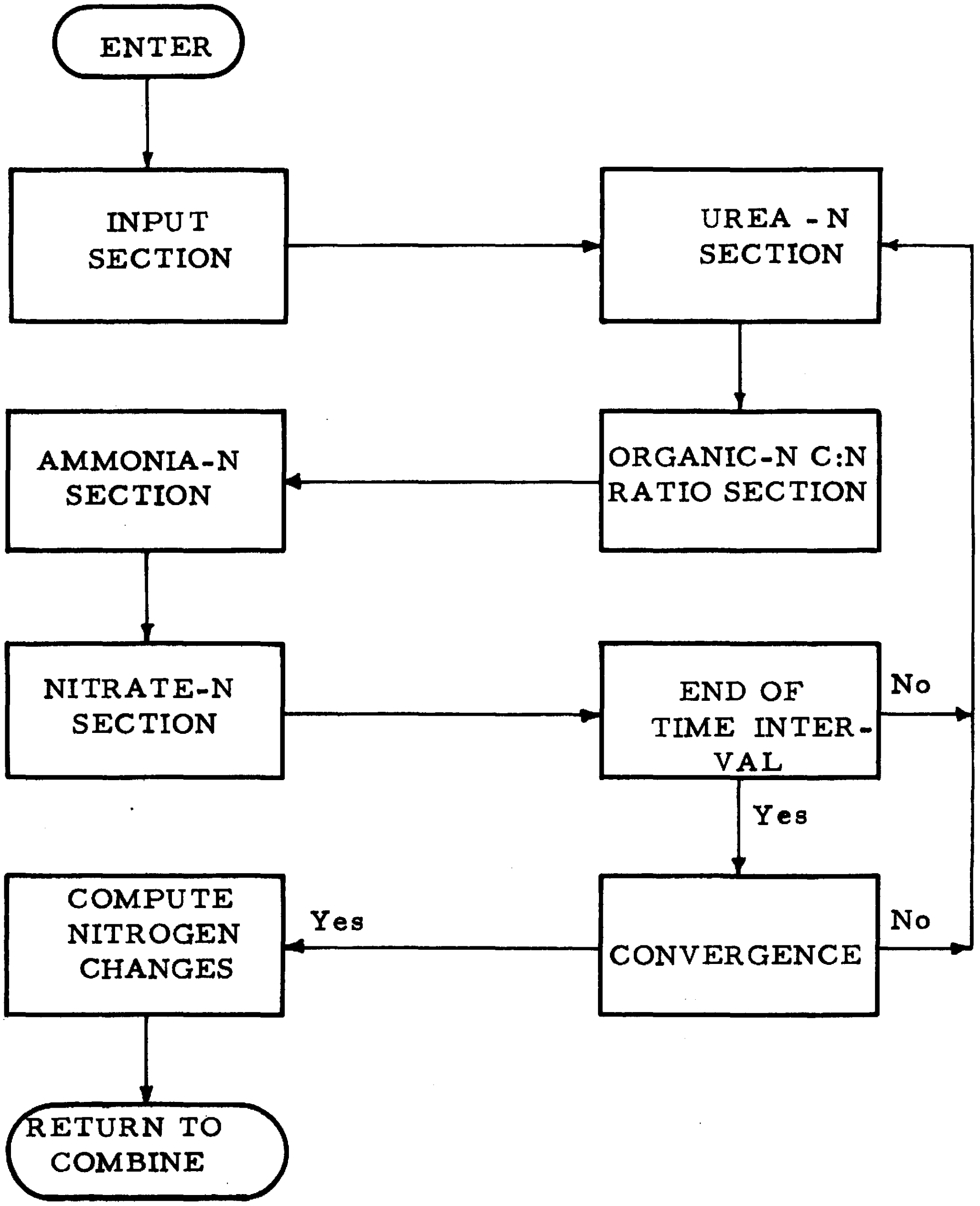


Figure 18A. Generalized block diagram of subroutine TRNSFM. (After Dutt et al. 1972)

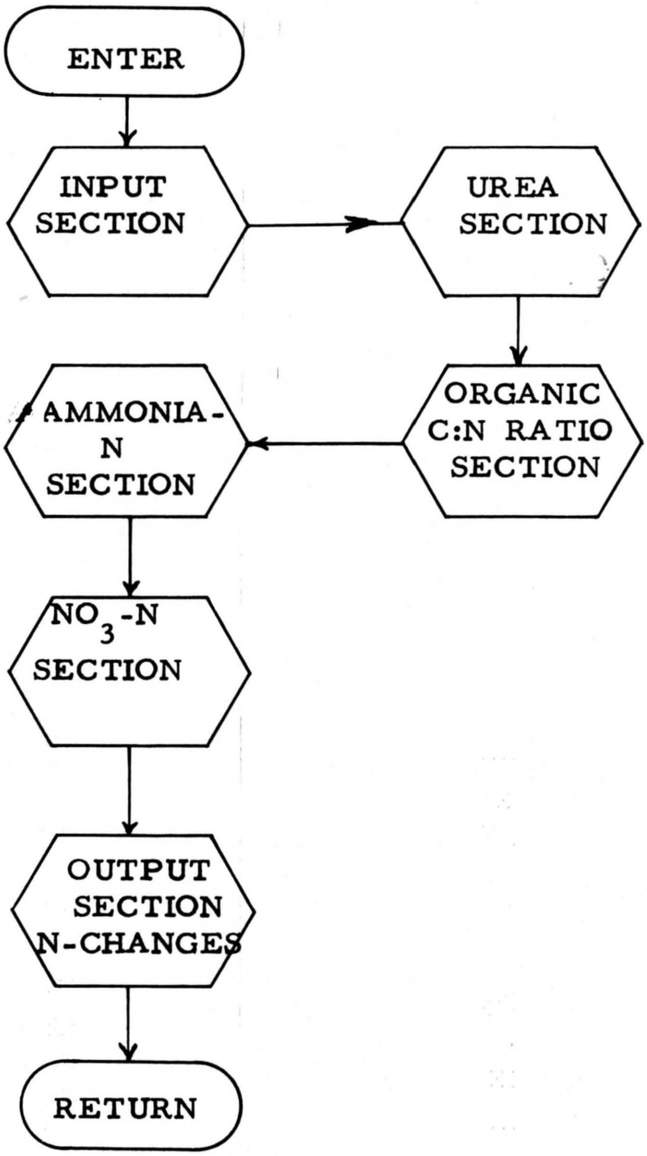


Figure 18B. Generalized block diagram of subroutine TRNSFM.

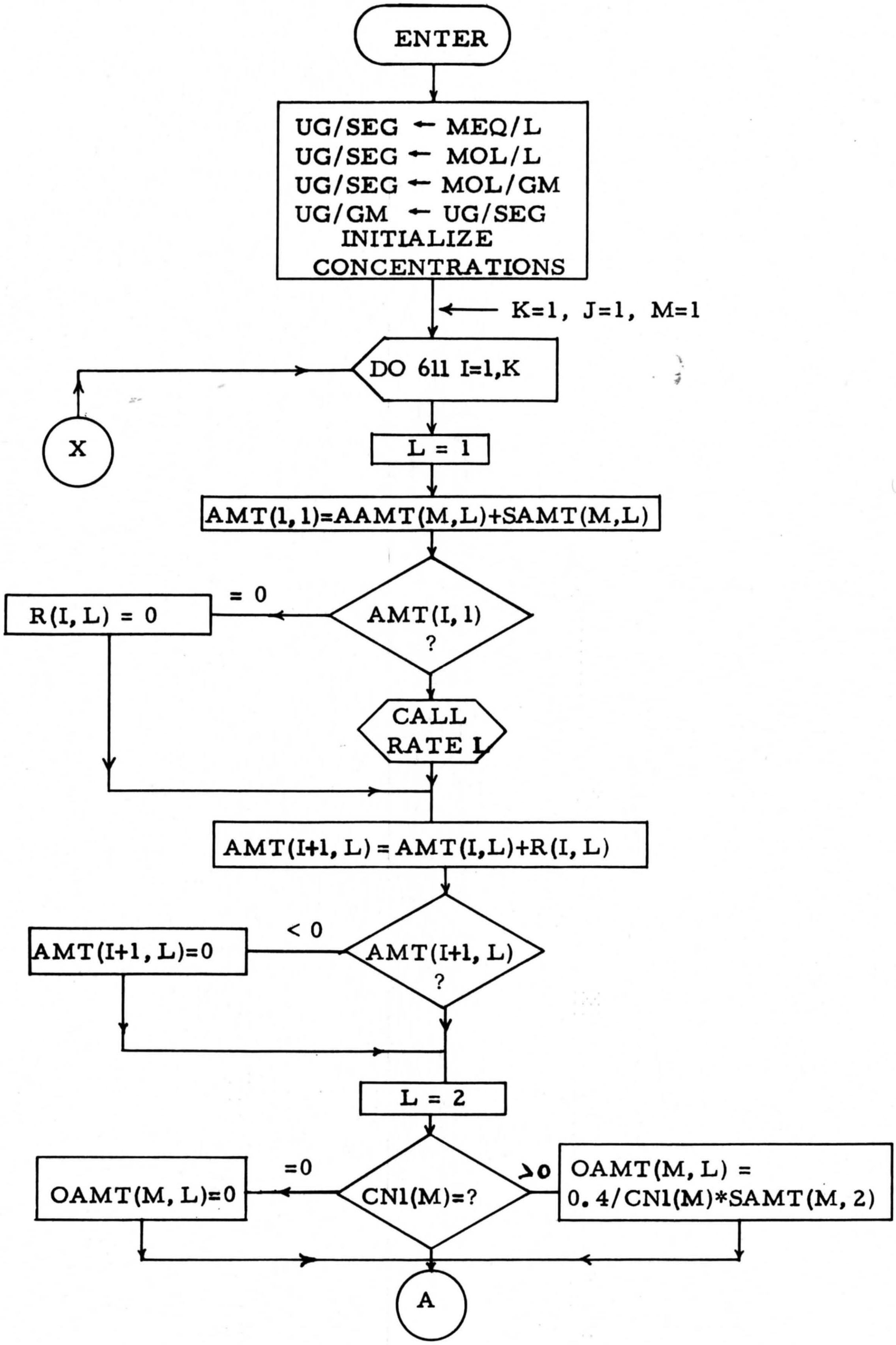


Figure 19. Flow chart of subroutine TRNSFM.

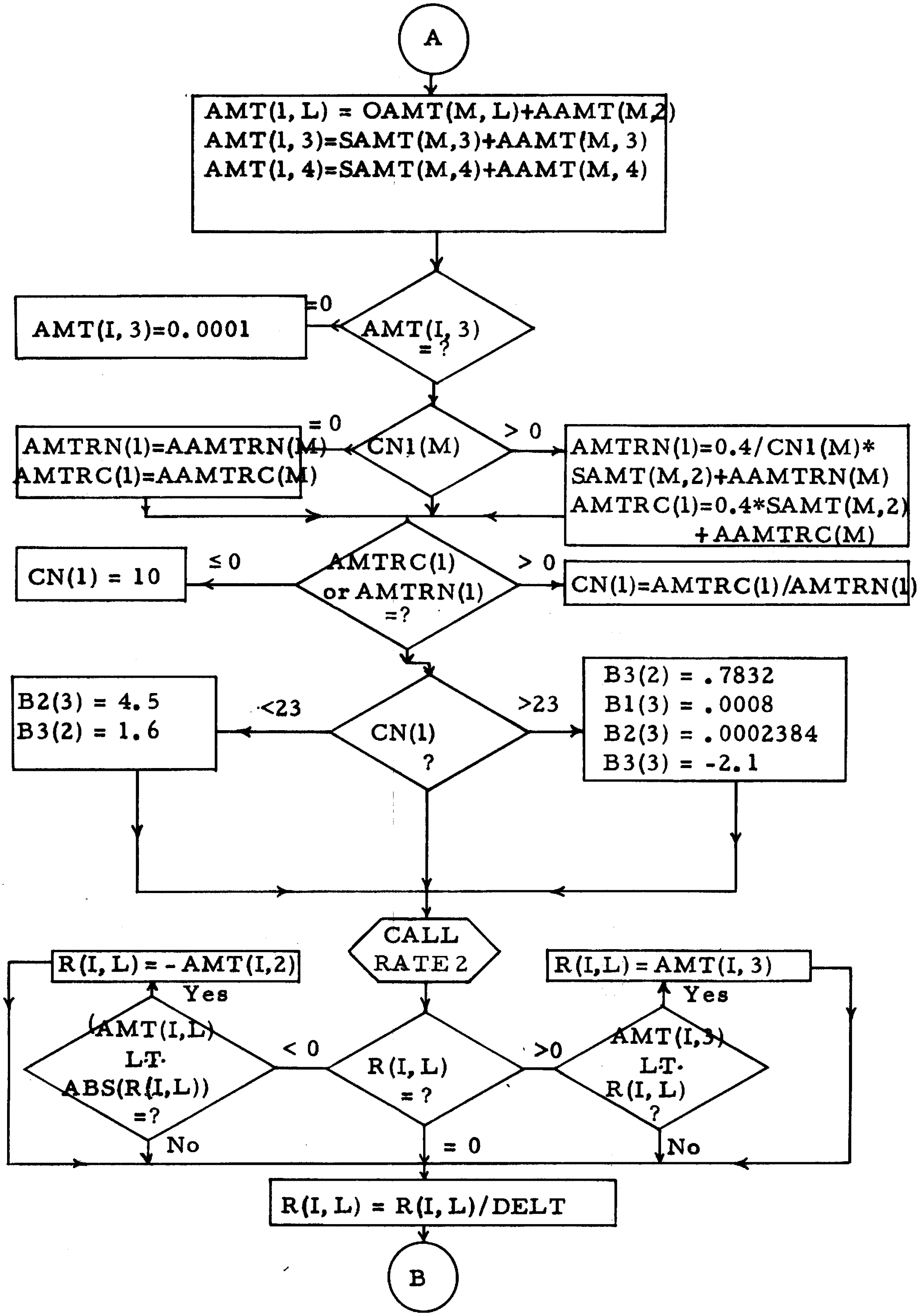


Figure 19. Flow chart of subroutine TRNSFM. (Continued)

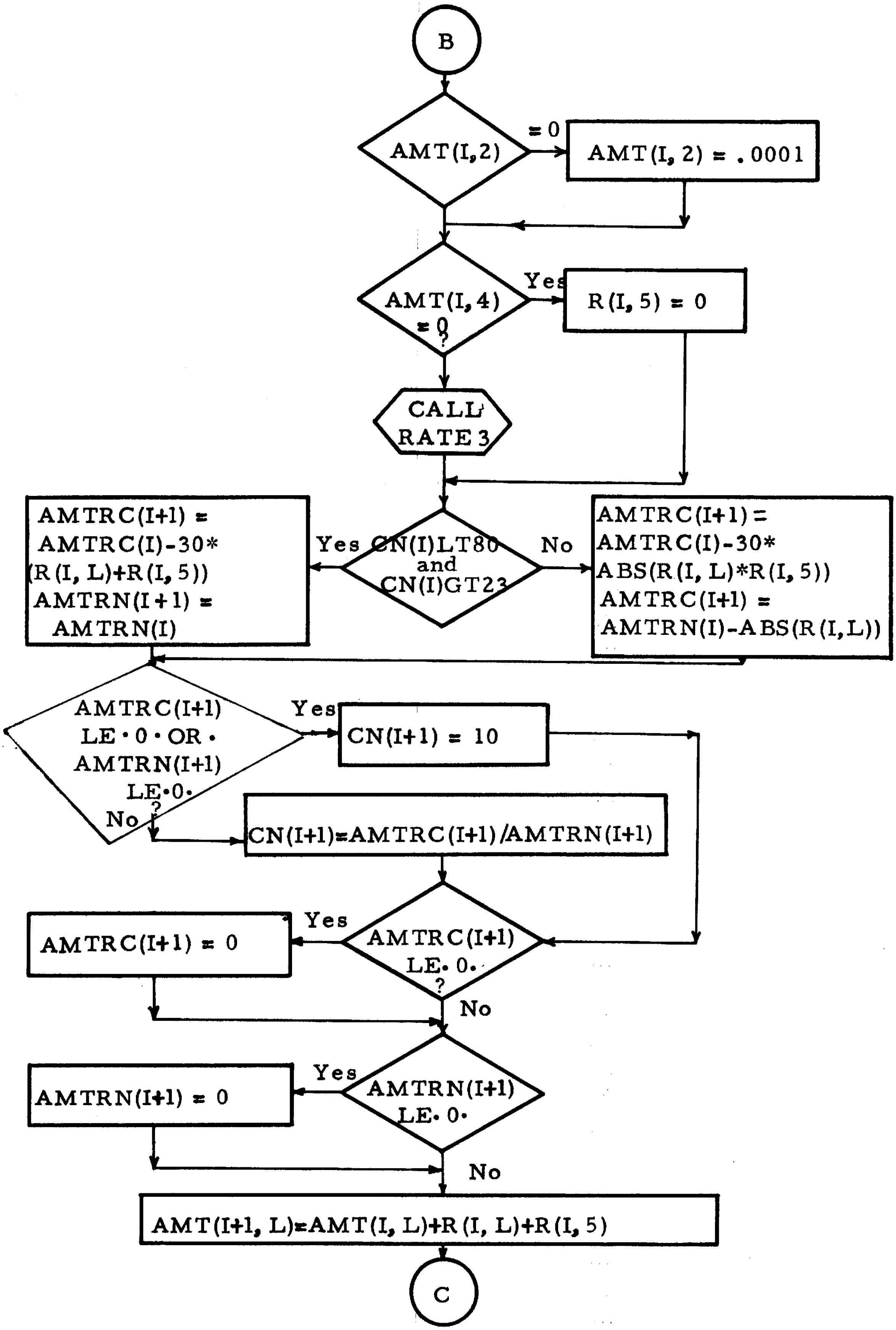


Figure 19. Flow chart of subroutine TRNSFM. (Continued)
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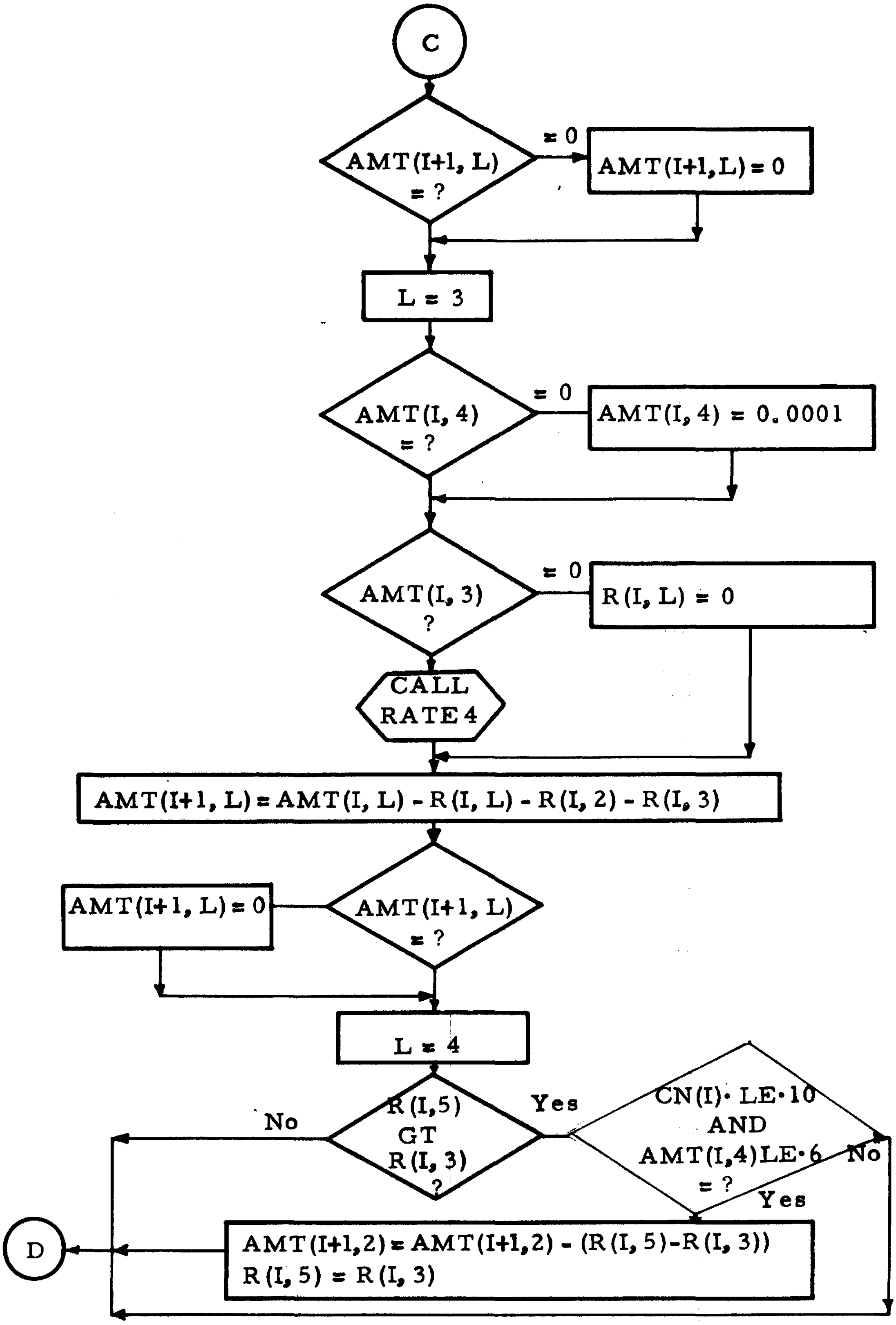

Figure 19. Flow chart of subroutine TRNSFM. (Continued)

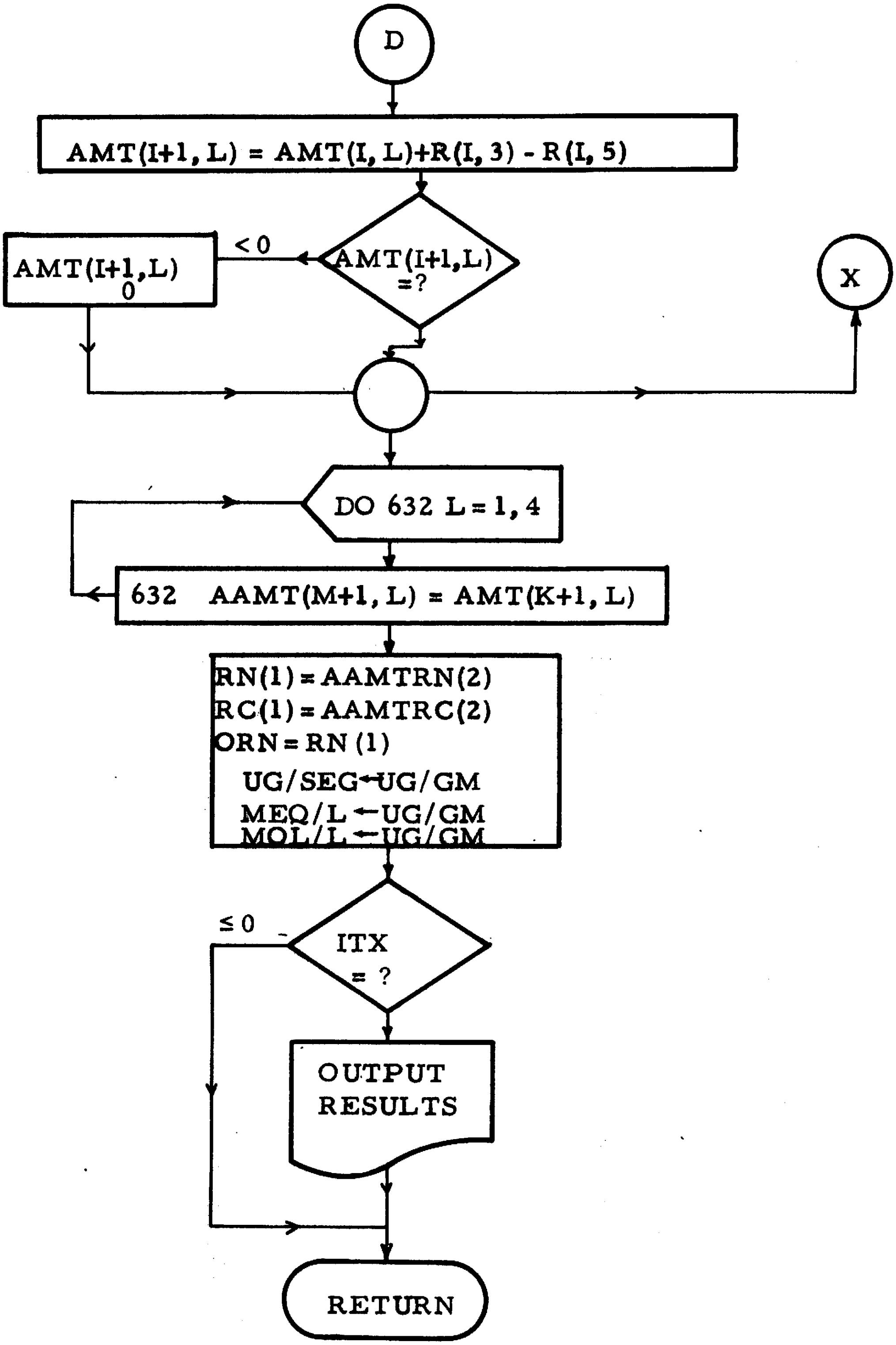

Figure 19. Flow chart of subroutine TRNSFM. (Continued)

in which they are arranged in the subroutine makes no difference in program operation.

The input section in Figure 18b is concerned with establishing basic constants, and control and input data. Unit conversions are done to convert amounts in ug/segment to ug/g soil and moisture tensions in cm of H_2O to bars. NO_3^- and NH_4^+ are converted from meq/l to ug/g soil.

The urea-N section includes routines for the initial time interval length and the initial concentration of urea-N. Also, the urea hydrolysis rate equation, an expression to compute the amount of urea-N present at the start of the next time interval, special logarithmic rate functions at limiting temperatures and urea-N concentrations, and other control loops are included in this subroutine section. The computer passes completely through this section before proceeding to the next.

The organic-N -C:N ratio section is the most involved part of the program. The initial parts are concerned with the concentrations of organic-N, NH_4^+ - N, and NO_3^- - N present at the start of a time interval. These data are necessary for the first set of calculations pertaining to an interval. After this, the data for the remaining time increments are generated entirely by the subroutine.

After establishing the initial C:N ratio range, the program enters the mineralization-immobilization rate equation. The resulting rate is modified according to the C:N ratio and the limiting temperatures, moistures, and concentrations.

Next is the NO_3^- - N immobilization rate equation. It is used at this point so that its results can be used along with the output from the mineralization-immobilization equation to calculate the C:N ratio at the start of the next time interval. Loops concerned with the limiting temperatures, moistures, and concentrations follow the equation.

The C:N ratio is recalculated in the routine which follows. Separate loops are used for the C:N ratio ranges greater than 23 and less than or equal to 23. The basic method of recalculation has already been described in Chapter III. The last part of the organic-N-C:N ratio section is concerned with storing the amounts of residue carbon and nitrogen present at the end of a call and computing the amount of organic-N present at the start of the next time increment.

The NH_4^+ - N section of the program contains the nitrification rate equation along with the appropriate limiting rate functions and control loops. Again, the last part is concerned with the computation of the amount of NH_4^+ - N present at the next time interval. The NO_3^- - N section is rather short since the appropriate rates have already been calculated. The routine computes the amount of NO_3^--N present at the start of the next time interval based on the initial amount of NO_3^- - N and the output from the nitrification and NO_3^- - N immobilization equations.

Rate adjustments for time

All the basic rates of transformations are in ppm/day. These rates are adjusted for the monthly time increments assuming linear relationship. This assumption is considered adequate in terms of this gross model, and this procedure seemed to work well for the overall system envisioned in this study.

The output area converts the value from ug/g soil to ug/segment. NO_3^- and NH_4^+ are, however, converted from ug/g soil to meq/l in solution.

CHAPTER VI

MODEL VERIFICATION

Introduction

Verification of a simulation model is performed in two phases, namely calibration, or parameter identification, and testing of the model. Both the phases of verification process require data from the prototype system. The hydro-quality (salinity) model described in the previous chapters is calibrated by applying it to the Snake River basin at Twin Falls, Idaho. The calibration is done by adjusting the various parameters in the equations used to describe the system, until known output functions are accurately duplicated. While the data for a period of one year is used for calibration purposes, the model is tested over the second consecutive year using an independent set of data to determine the level of agreement between the observed and computed output functions. This chapter relates to the results of verification of the model with the prototype.

Choice of Prototype

The hydro-salinity model was applied to a large irrigated area of the Snake River Plains in the vicinity of Twin Falls, Idaho (Figure 1). The reasons for selecting this area for verifying of the model are as follows:

1. Adequate hydrologic and salinity data for this area are available for the period October 1968--September 1970. These data have been collected and processed by the Snake River Conservation Research Center at Kimberly, Idaho.
2. Water and salt balances have already been achieved on an annual basis for this area for the period October 1968 -- September 1970 (Carter et al., 1971).
3. Also, the application of the model to this area provided a good opportunity to evaluate its performance, particularly under conditions where groundwater flow is predominant, and to improve the capability of the model as required.

Details of Prototype Basin

The information contained in the following section is adopted from Carter et al. (1971 and 1973).

Development of the area

The study area (Figure 1) was developed by the Twin Falls Canal Company and has been under irrigation for about 65 years. Soon after irrigation, high water tables appeared in localized areas throughout the tract. To alleviate this problem about 50 tunnels were excavated into the basalt rock underlying the high water table areas. These tunnels were terminated when fractures in the rock carrying significant amounts of water were intercepted. The tunnels then served as effective drainage channels to convey excess water into natural surface drains for some time. Since the year 1930 some tile relief wells were also excavated. The flow into the wells is by hydrostatic pressure. Water from wells is connected to natural surface channels by tile lines. All the surface and subsurface drainage returns to the Snake River, which flows through a canyon about 500 ft. deep forming the northern boundary of the project.

Water use pattern

Water is diverted from the Snake River to the study area and allocated to farmers at the rate of approximately 0.5 cubic feet/sec for each 40 acres continuously. Water is in the canal system from about April 1 to November 15 each year. Canal flows in the early spring and late fall are considerably lower than during the peak irrigation season of June, July, and August because some crops do not require early spring and late fall irrigation.

Soils and geology

Soils of the study area are wind deposited, calcareous, silt loams, ranging from 0 to 15 m (0-50 feet) deep. A caliche and silica cemented hardpan layer is found from 0.30 to 0.45 m (12 to 18 in.) below the surface over most of the area. The soils are underlain by fractured basalt to depths of several hundred meters. Water infiltration rates are fairly high and most crops are irrigated by small furrows.

Vegetation and cropping pattern

The most important crops are alfalfa, dry beans, sugarbeets, small grain, corn, and pasture. The row crops are normally seeded in April and May, and normally the last crop harvested is sugarbeets, which is generally in October. Crop rotation also is practiced, but the relative acreages remained essentially the same.

Sources of Data

Climatological data

Precipitation and temperature records for the three stations Kimberly, Twin Falls, and Buhl are obtained from the Weather Bureau stations for the period of study.

Streamflow, canal diversions and groundwater data

Sampling sites selected throughout the area included the project diversion at Milner Dam on the Snake River, 15 drainage tunnel outlets, five tile-relief well network outlets, four main natural surface drains (Rock Creek, Cedar Draw, Mud Creek, and Deep Creek), and approximately 15 small natural surface drains returning water to the Snake River. These sites, except the small surface drains, are shown in Figure 1 by number. Water stage recording stations were maintained on the main surface drains. Existing U. S. Geological Survey gaging stations were utilized on Cedar Draw and Deep Creek. New gaging stations were established on Lower Rock Creek and Mud

Creek. Measurements from tile relief well network outlets and from the drainage tunnel outlets constituted the groundwater measurements for this study. Samples from each site, except the 15 small natural surface drains, were collected at 2-week intervals for the Canal Company water year, October 1, 1968, through September 30, 1969. Surface runoff water samples were collected at irregular intervals during the study year. The record of water diverted was provided by the Twin Falls Canal Company in cooperation with the U.S. Geological Survey.

Quality data

Water samples were collected at 2-week intervals for analysis from all sampling sites. Samples were analyzed for Na^+, K^+, Ca^{++}, Mg^{++}, Cl^-, HCO_3^-, $SO_4^=$-S, $PO_4^\equiv$-P, and NO_3^--N concentrations. After analyzing all samples for all components for a few months, it was found that the concentrations of some components were nearly constant. Therefore, only $PO_4^\equiv$-P, NO_3^--N, total salt concentrations, and water temperature at the site were continued at 2-week intervals. Analyses for other components were made at 4-week intervals. After 18 months, sampling was discontinued at some sites. The remaining sites were samples for one more year at monthly intervals, and the samples analyzed for all components. Concentrations of the various components were determined in surface runoff water at a number of sites throughout the tract.

Table 7 shows a typical analysis of water samples in the study area. Data on soils was not current for the period of study. Available data from the SCS and the University of Idaho was used in the study. Crop uptake of N and organic matter turned into soil were estimated on an annual basis. Monthly values were further estimated from these annual figures. Average quantities of fertilizer applications have been assessed based on local inquiries.

Results

Hydrology model

Since water quality and quantity are two interrelated dimensions, accuracy in quality dimension calls for a corresponding accuracy in the predicted quantity of flow. The problem is of concern in return flow systems where subsurface flow is significant. This will, therefore, require a better understanding and adequate representation of the components of the system. The prototype system of this study has a significant amount of subsurface flow contributing to surface runoff.

The following discussion is adopted from Carter et al. (1971), in respect to behavior of drainage tunnels and subsurface return flow.

> "Normal flow in these drains from December through March consisted of only subsurface drainage water from tunnels from tile-relief well networks. Canal company records and flow measurements showed that the subsurface drainage flows from these sources cycle yearly, with maximums in the fall and minimums in the spring."

Table 7. Typical analysis of water samples in the study area.

Ion	Concentration in Meq/l	Ion	Concentration in Meq/l
A. Diversion water (inflow)			
Ca^{++}	2.54	Cl^{-}	0.66
Mg^{++}	1.23	HCO_3^{-}	3.38
Na^{+}	0.90	NO_3^{-}	0.0086
K^{+}	0.12	$SO_4^{=}$	0.91
	4.79		4.9586
B. Subsurface drainage water			
Ca^{++}	4.27	Cl^{-}	1.52
Mg^{++}	3.14	HCO_3^{-}	6.61
Na^{+}	3.67	NO_3^{-}	0.23
K^{+}	0.15	$SO_4^{=}$	3.00
	11.23		11.36
C. Runoff water (Oct. 1969)			
Ca^{++}	3.44	Cl^{-}	0.80
Mg^{++}	2.30	HCO_3^{-}	5.46
Na^{+}	2.34	NO_3^{-}	0.052
K^{+}	0.16	$SO_4^{=}$	1.05
	8.24		7.362

The yearly cycling of flow suggested adoption of a time variant parameter for the subsurface contribution to the total surface runoff. Calibration of the hydrologic model, therefore, considered both the time variant and fixed aparameters. Table 8 shows a list of time invariant parameters (both digital and analog) and their optimum values obtained during the parametric identification process. Time variant parameters of importance are (1) the percentage of subsurface runoff contributing to surface outflow, FK, and (2) water application and conveyance efficiency of the system, EFF.

The entire calibration procedure consisted of adopting both the self calibration technique adopted by Hill et al. (1973) and manual calibration adopted by Thomas (1971). This was required because both time variant and fixed parameters were considered in the model. Represented by Figure 20 is a typical distribution showing the percentage of subsurface flow contributing to surface outflow. A typical time variant distribution is also obtained in respect to efficiency of water application, and is shown in Figure 21. The computed and observed quantities of return flow are, however, shown in Figure 22. The correlation between computed and observed outflows is high, with a correlation coefficient near 0.96. Appendix E contains the computer output of the hydrologic model of the system for water years 1968-1969.

Table 8. Optimum time invariant parameters of hydrology model.

(A) DIGITAL PARAMETERS (DIG)

	Mnemonic	Description	Optimum Value
1	SNO	Initial water equivalent of snow pack	0.0
2	FMES	Critical moisture content	4.0
3	FMCS	Field capacity	8.0
4	SMC	Snow melt coefficient	0.12
5	SPC	Outflow constant to correlate ungaged inflow with snow melt	0.70
6	FMIN	Initial moisture content	8.00
7	AGINIC	Initial quantity of Ag. outflow	7.50
8	T	Delay time of subsurface flow (months)	3.0

(B) ANALOG PARAMETERS (PH)

	Mnemonic	Description	Optimum Value
1	C_2	Constant to correlate ungaged flow to (SNMLT + PRE)	0.0
2	C_1	Constant to correlate ungaged flow to (SNMLT + PRE)	0.01
3	FMCS /SKAL	Scaled field capacity	0.40
4	QGTIC/SKAL	Scaled initial subsurface flow	0.375
5	C_4	Ungaged surface flow correlated to canal diversions	0.0
6	C_3	Ungaged surface flow correlated to canal diversions	0.01
7		Initial ground water inflow	.001
8	C_6	Ungaged ground water inflow correlated with (PRE + SNMLT)	.001
9	C_5	Ungaged ground water inflow correlated with (PRE + SNMLT)	.001
10	$1/kg_2$	Ground water delay sequence correlated to inflow	.001

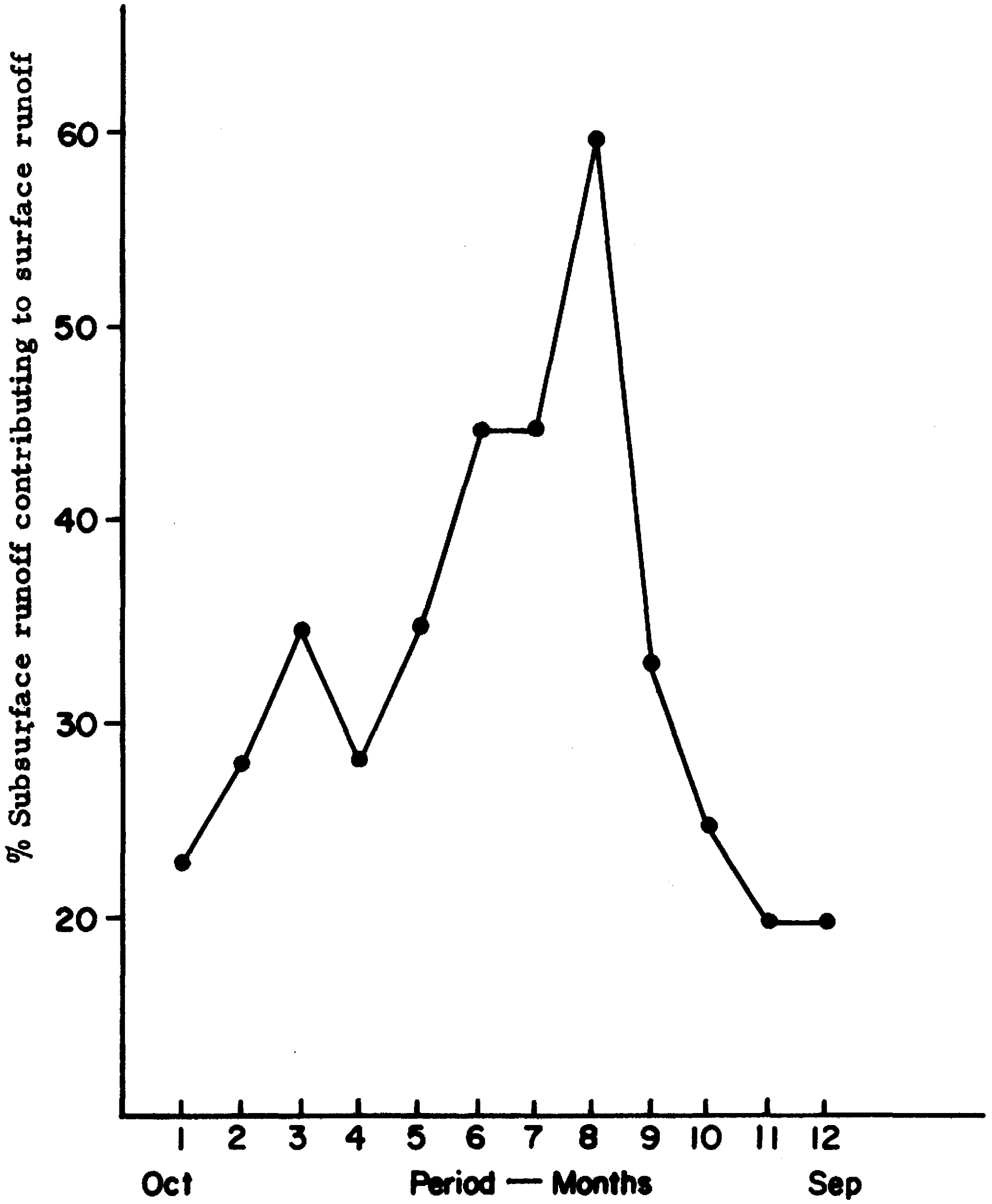

Figure 20. Typical distribution of percent subsurface flow contributing to surface runoff.

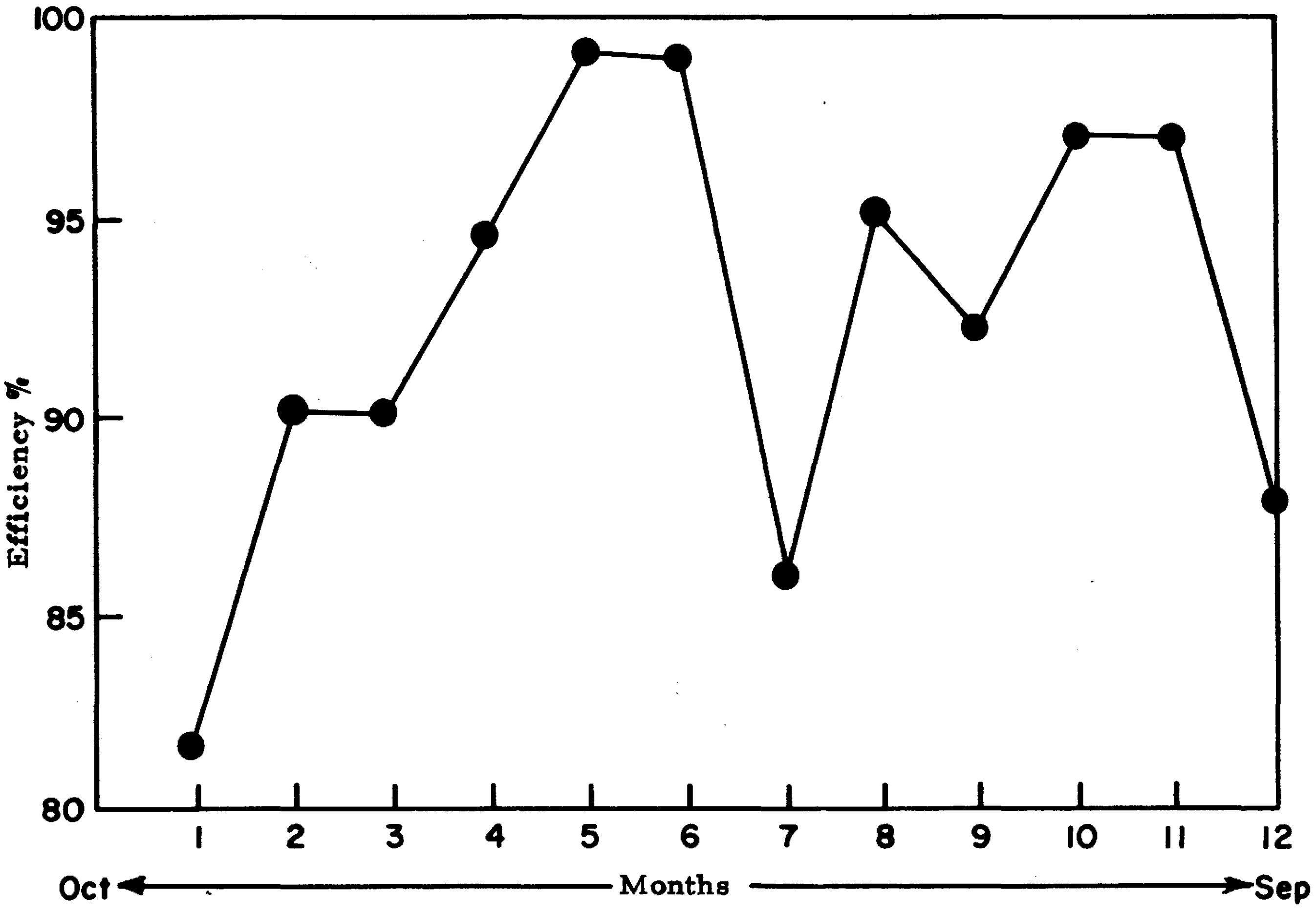

Figure 21. Typical distribution of efficiency of water application.

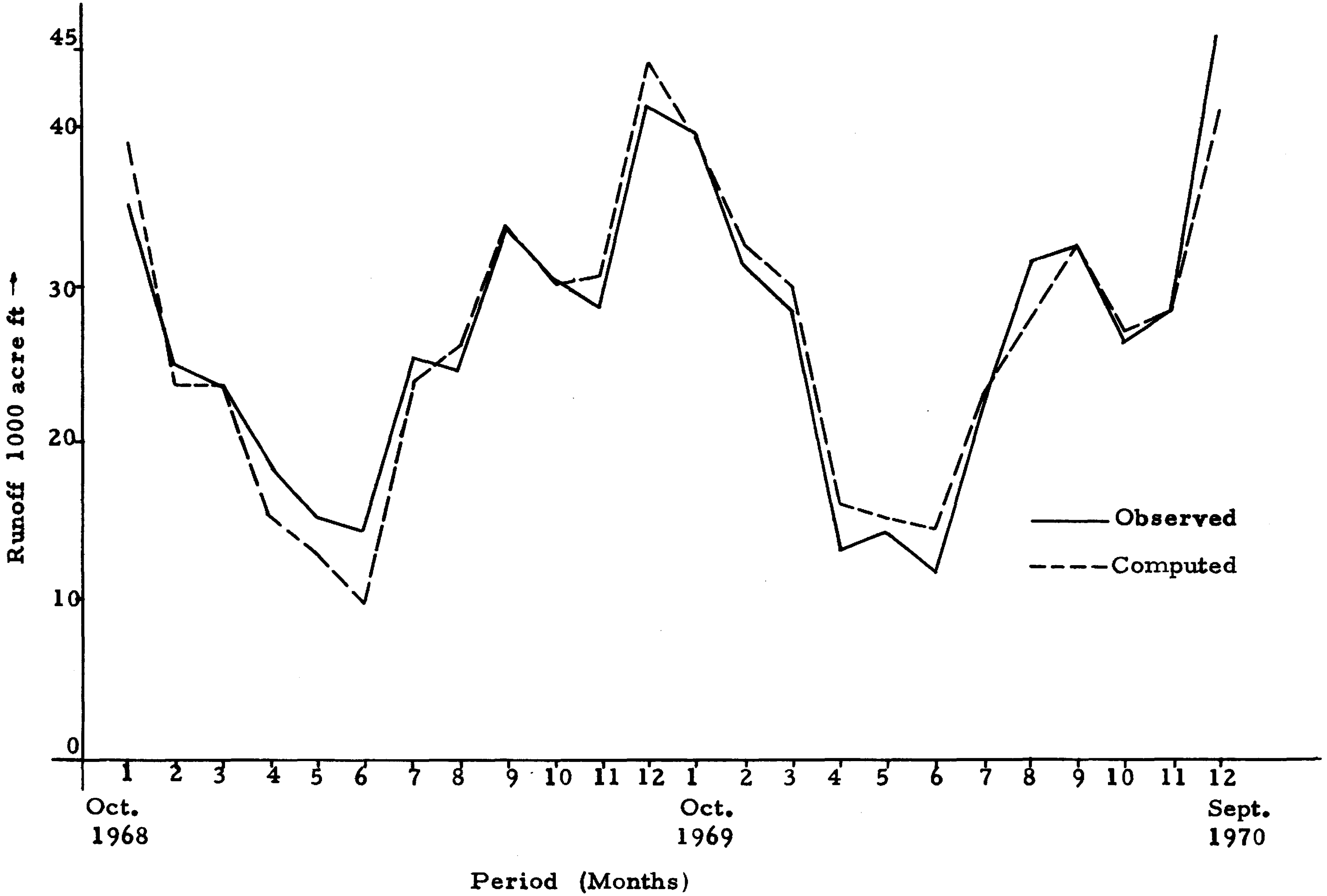

Figure 22. Monthly runoff computed vs. observed.

Chemical and biological models

Since the chemical and biological subsystems are intensively interconnected, the results discussed herein pertain to the combined effect of both these models. The concentrations of each of the ions Ca^{++}, Mg^{++}, Na^{+}, Cl^{-}, $SO_4^{=}$, HCO_3^{-}, and NO_3^{-} are predicted. In arriving at the results, the initial concentrations of ions in the soil solution played an important role, unlike the hydrology model. In this study, the initial concentrations of ions in the soil water have been estimated. The estimation is by trial and error based on the results of soil analysis (for the top 6 feet of soil) conducted by the University of Idaho a few years back. The concentrations of individual ions have been estimated with the following considerations.

1. It has been found that large areas consisted of a hard layer of caliche of varying thickness. The subsurface water from the drainage tunnel outlets has different levels of concentrations indicating a spatial variability of the ionic concentrations. The model area has, therefore, been divided into two sectors to represent different levels of concentrations of ions in the soil water, and within the fissures of basalt through which the water percolates.
2. The carbonate water in the soil is assumed to have a higher partial pressure of CO_2 compared to the atmospheric value, with consequent increase in concentration of HCO_3^{-}.

3. Weathering of the calcic plagioclase portion of the basalt releases more sodium, resulting in a high concentration of sodium in the soil water system.
4. Presence of gypsum has not been assumed.

The initial ionic concentration of soil water finally adopted in the calibration of the model is presented by Table 9. The results of the chemical quality of the return flow are discussed below with respect to individual ions comprising the total salts.

Calcium. Calcium ion accounted for about 11 percent of the total effluent salts. Predicted concentrations of calcium in the subsurface runoff are within the range 4.78 - 3.07 meq/l. These values are in agreement with the corresponding observed concentrations (Carter et al., 1973) at the drainage tunnels. The variations in the concentrations may be attributable to different depths of water percolation in the soil before being tapped by drainage tunnels. Deeper percolation may have lesser and uniform concentrations as much of the CO_2 in the soil water may have been used up to form HCO_3^-. Shown by Figure 23 are the computed and observed runoff of calcium ion in tons. For the two year period computed calcium averaged approximately 11 percent less than the measured outflow, with a correlation coefficient of 0.89, n = 24.

Magnesium. The predicted concentrations of magnesium ion in the subsurface runoff are in agreement with the observed values

Table 9. Initial values of ionic concentrations in soil water.

Soil Layer	Meq/l								CEC meg/ 100 gm	Lime Moles /gm	Gyp-sum	Soil Type
	Ca	Mg	N	K	HCO_3	CL	SO_4	NO_3				
1	1.50	1.20	10.0	0.11	10.0	1.40	1.50	0.50	12.5	3.0	0	1
2-15	1.50	1.20	10.0	0.11	10.0	1.40	1.50	0.25	12.5	3.0	0	1
1	2.50	2.0	12.5	0.11	11.5	1.40	4.0	0.50	12.5	3.0	0	2
2-15	2.50	2.0	12.5	0.11	11.5	1.40	4.0	0.25	12.5	3.0	0	2

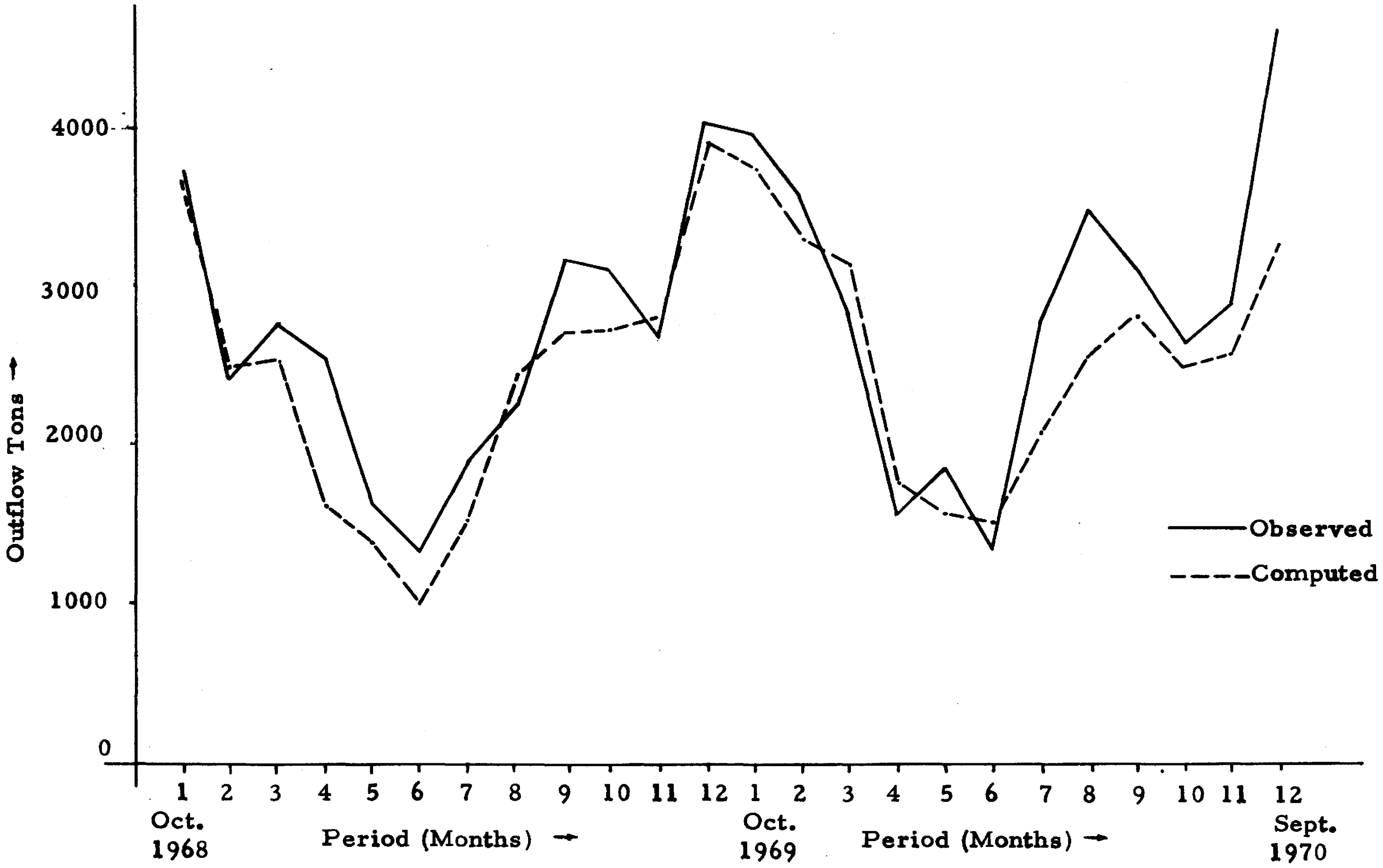

Figure 23. Observed and simulated calcium (Ca^{++}) outflow.

and are within the range 3.92 - 2.51 meq/l. Figure 24 represents the computed and observed quantities of magnesium ion in the runoff. The computed quantity averaged approximately 6 percent more than the measured flow, with a correlation coefficient of 0.87, n = 24.

Chloride. Chloride ion has minimum variation in concentrations both in the computed and observed subsurface runoff. Figure 25 illustrates the computed and observed quantities of chloride, having a correlation coefficient of 0.78, n = 24.

Sodium. Sodium ion, like calcium, varies in concentrations in the subsurface runoff. The computed values are within the range 3.78 - 2.96 meq/l and compare well with the observed values of concentrations in the drainage tunnels. Figure 26 illustrates the computed and observed quantities of sodium. The correlation coefficient is 0.84, n = 24.

Sulphate. Sulphate ion accounted for about 14 percent of the total effluent salts. The range in computed concentrations of this ion in the subsurface runoff is 3.15 - 1.31 meq/l, while that of the observed values in drainage tunnels is 5.0 - 1.2 meq/l. The variation in the computed and observed concentrations is probably a result of not considering more complex ion pair formations of sulphate with other ions, like $NaSO_4^{-1}$, in the equilibrium calculations, and also due to difficulty in assessment of initial concentrations in the absence of actual data. Figure 27 shows the computed and observed quantities

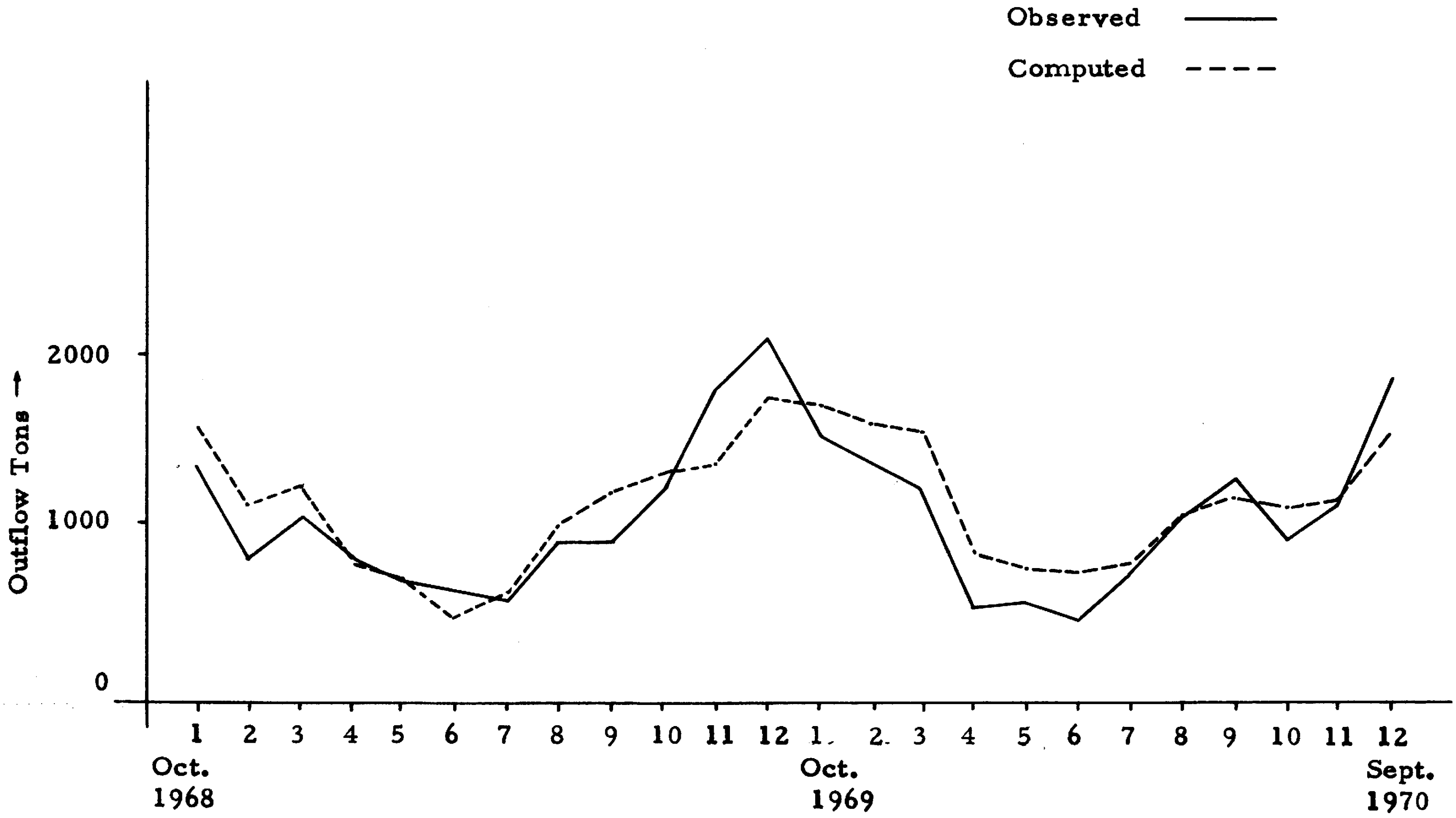

Figure 24. Observed and simulated magnesium (Mg^{++}) outflow.

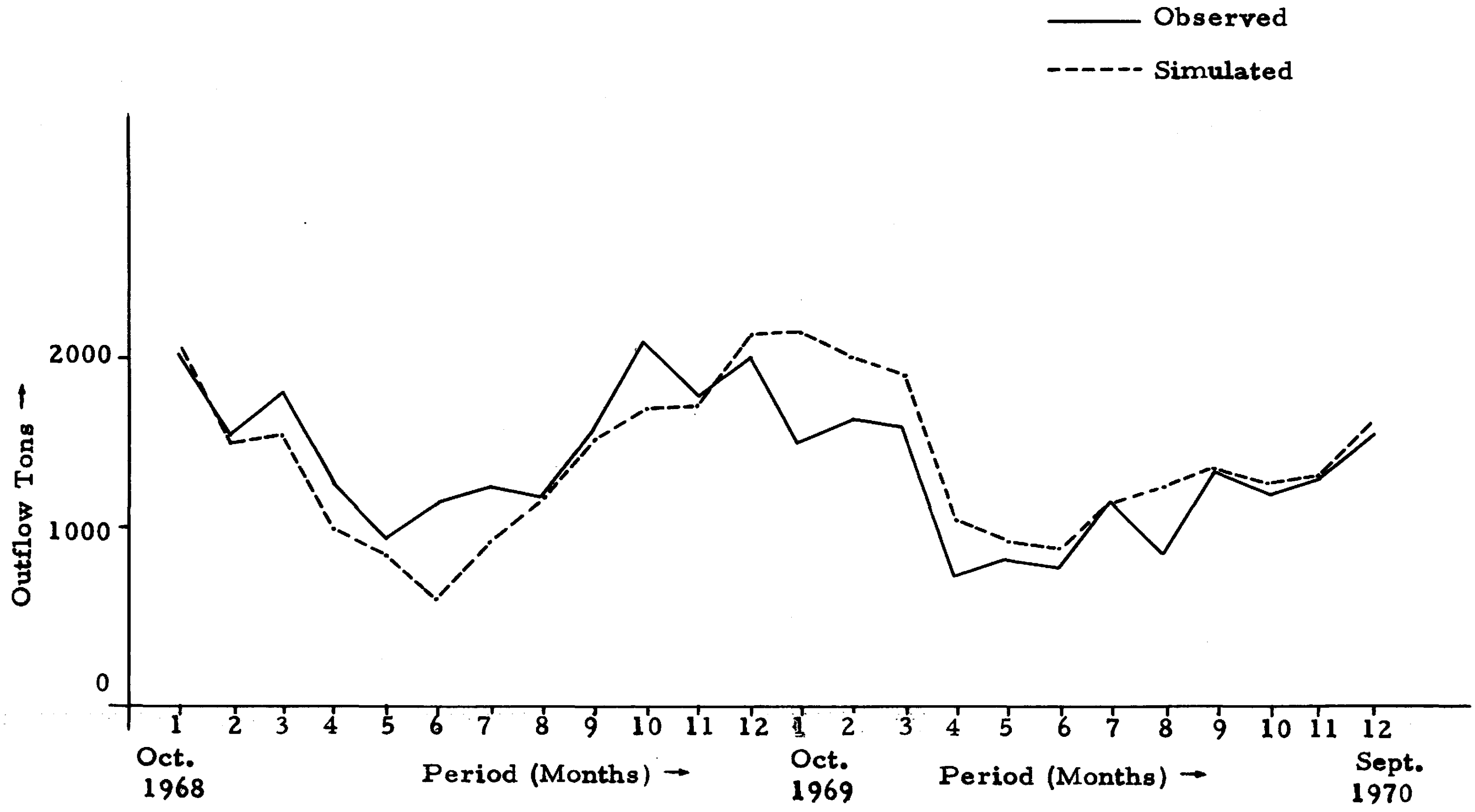

Figure 25. Observed and simulated chloride (Cl^-) outflow.

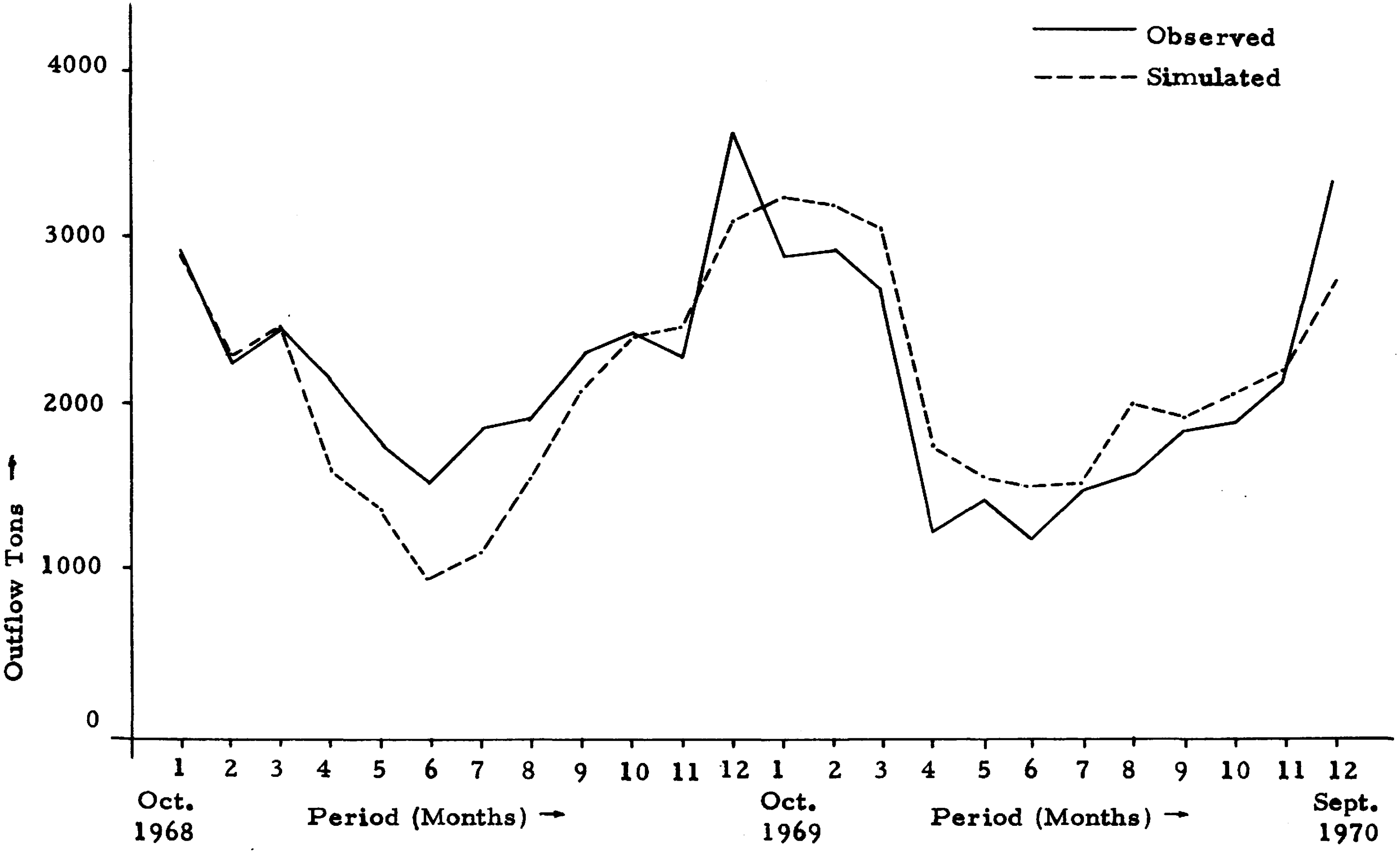

Figure 26. Observed and simulated sodium (Na^+) outflow.

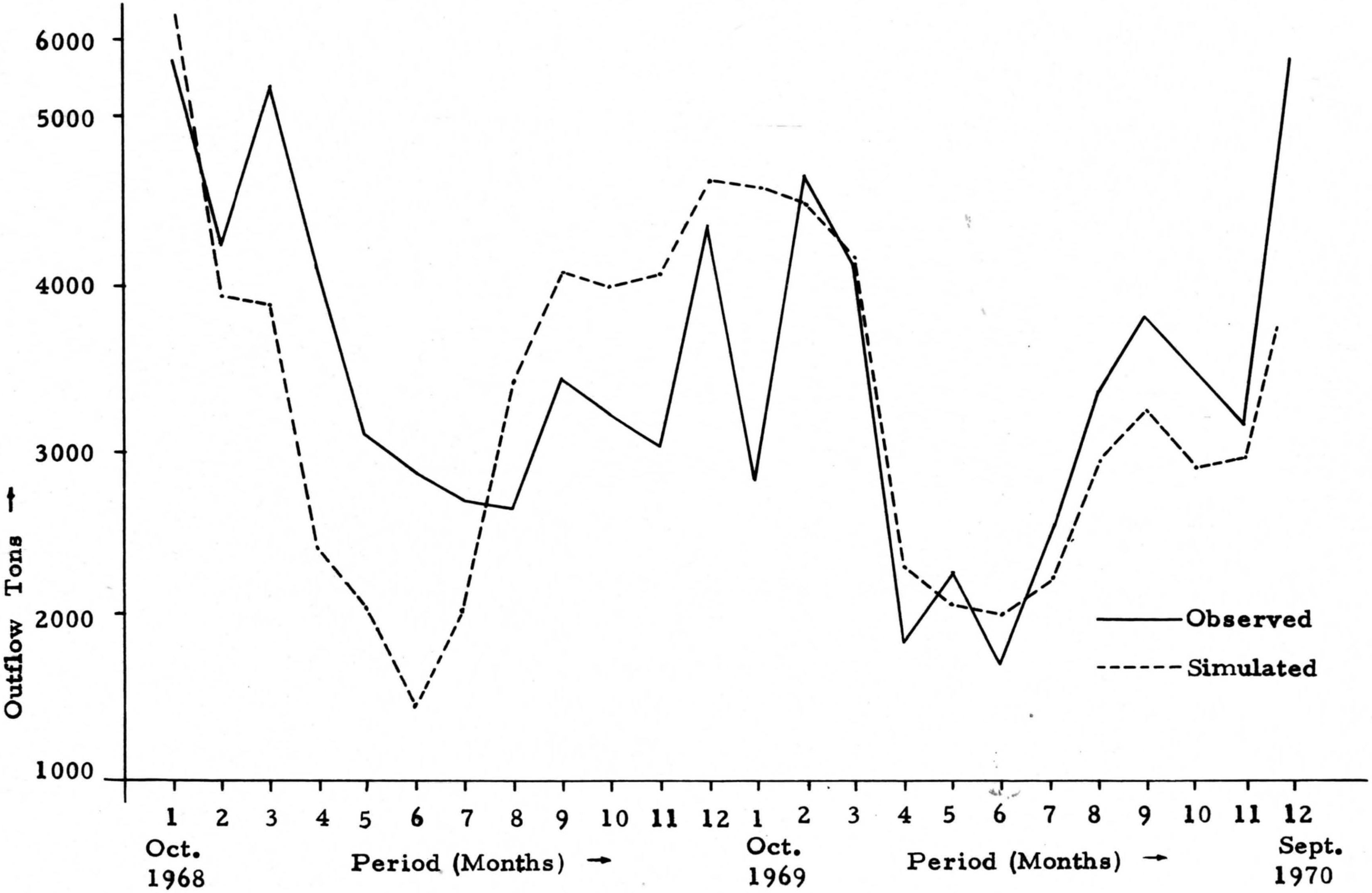

Figure 27. Observed and simulated sulphate ($SO_4^=$) outflow.

of sulphate in the runoff. It exhibits a poor fit during the calibration period with an overall correlation coefficient of 0.66, n = 24. The computed quantities of sulphate are low in the initial months and more in subsequent months of the calibration period of one year. The computed values have, however, a closer fit in the second year during which the model is tested. This is probably due to difficulty in establishing the initial conditions.

Bicarbonate. Bicarbonate ion accounted for about 52 percent of the total effluent salts. The computed concentrations of this ion in the subsurface runoff are 8.15 - 6.48 meq/l, and these values compare well with the observed values. The predicted and observed quantities of biocarbonate in the runoff are shown by Figure 28. While there is a good agreement during the calibration period, the computed quantities are slightly higher during the testing phase, giving an overall excess of approximately 7 percent when compared to measured quantity with a correlation coefficient of 0.89, n = 24. This is probably a result of difficulty in assessing the initial conditions.

Nitrate. Simulation of nitrate ion, a significant contribution in this study, accounted for a small fraction of the total observed salts, being less than 1 percent. However, the methodology of simulating this ion along with other ions in the subsurface runoff, illustrated the possible behavior of this ion in the overall system. The computed concentrations of nitrate in the subsurface runoff are 0.25 - 0.22 meq/l

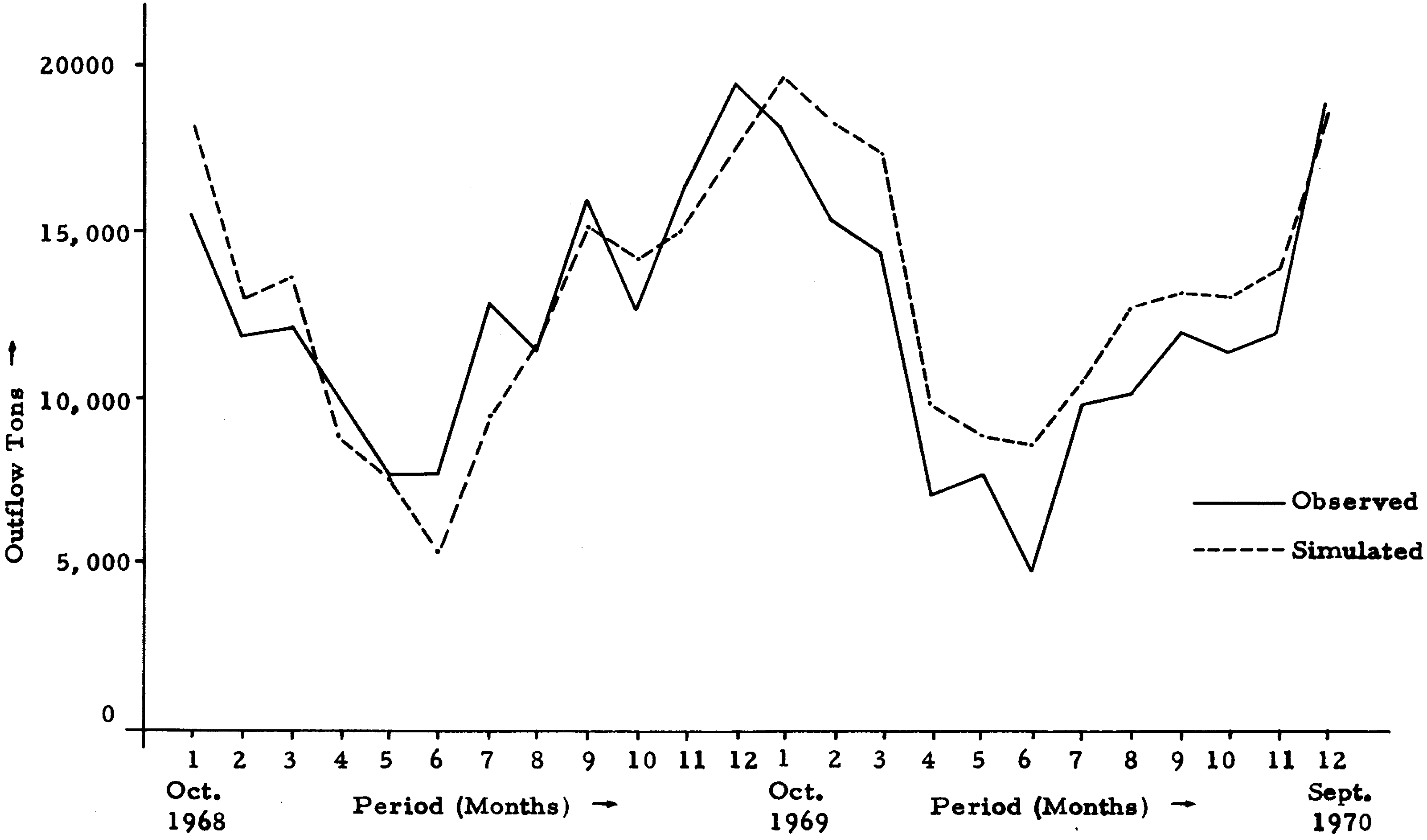

Figure 28. Observed and simulated bicarbonate (HCO_3^-) outflow.

while the observed values have a range of about 0.34 - 0.11 meq/l (Carter et al., 1973). The variations in the concentrations are probably a result of the following:

1. Assumptions made in the biological transformation model described in the preceding chapters.
2. Treating nitrate as a conservative parameter, similar to chloride.
3. Difficulty in estimating the initial concentrations in the soil solution.
4. Difficulty in estimating the fertilizer applications and nitrate uptake by growing plants within the time increment considered in the model.
5. Possibility of higher concentrations of nitrate in those drainage tunnels that intercept shallow soil profile.

Figure 29 shows the predicted and observed quantities of nitrate in the effluent waters, after considering the uptake by aquatic biomass within the surface channels of the runoff. (The uptake by aquatic biomass during the testing period is, however, assumed to have a linear variation with respect to temperature.) While there is a reasonably good fit during calibration period, the curve shows a porr fit during summer months. The variation in computed quantities may be a result of a possible change in management practices in the field with respect to quantity of biomass. It is likely that the quantity of biomass

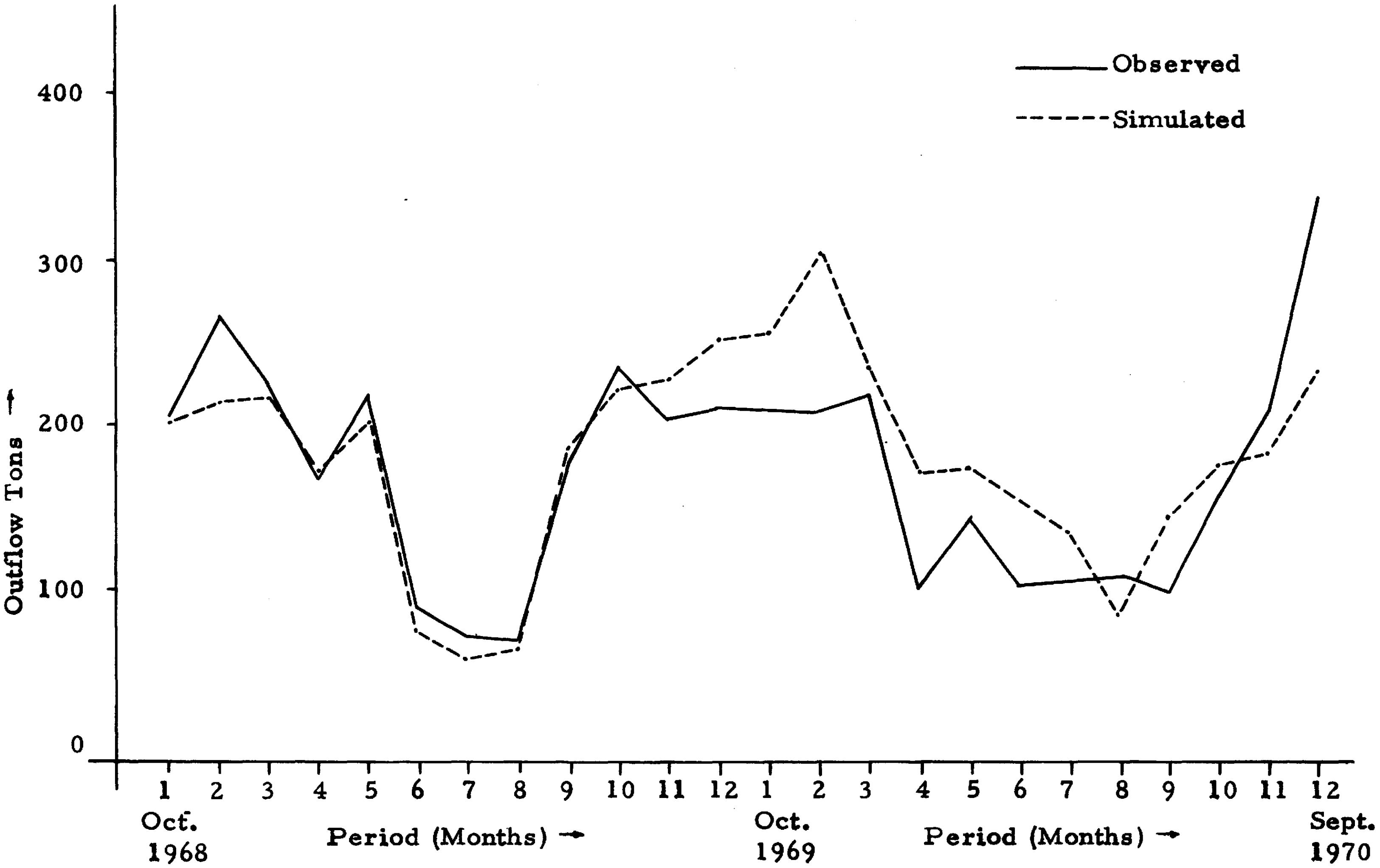

Figure 29. Observed and simulated Nitrate (NO_3^-) outflow.

is being altered during summer months (maybe in alternate years) on account of its profuse growth in these months. This practice will, therefore, yield higher quantities of nitrate in the surface runoff in the summer months. Further testing of the model is necessary to establish the extent of such cyclic changes in the management practices in the field. The correlation coefficient obtained is 0.81, n = 24.

Total dissolved solids. In this study the total dissolved solids is obtained by summation of individual ions. Figure 30 shows the observed and computed quantities of total dissolved solids. For the two years of study, the computed quantity of TDS is 2 percent higher than the corresponding observed value, with a correlation coefficient of 0.90, n = 24.

Model utility

Among the various uses the model can be put to is the study of the effects of alternative management practices on the quality of water. The particular management situations selected in order to demonstrate the utility of the model are discussed below.

Effects of changing composition of fertilizers: The type of fertilizers assumed in the calibration of the model were the urea and ammonium types in equal proportions. Under the assumed management situations the effect of applying only one type of fertilizer, namely urea, has been considered. A typical distribution of the

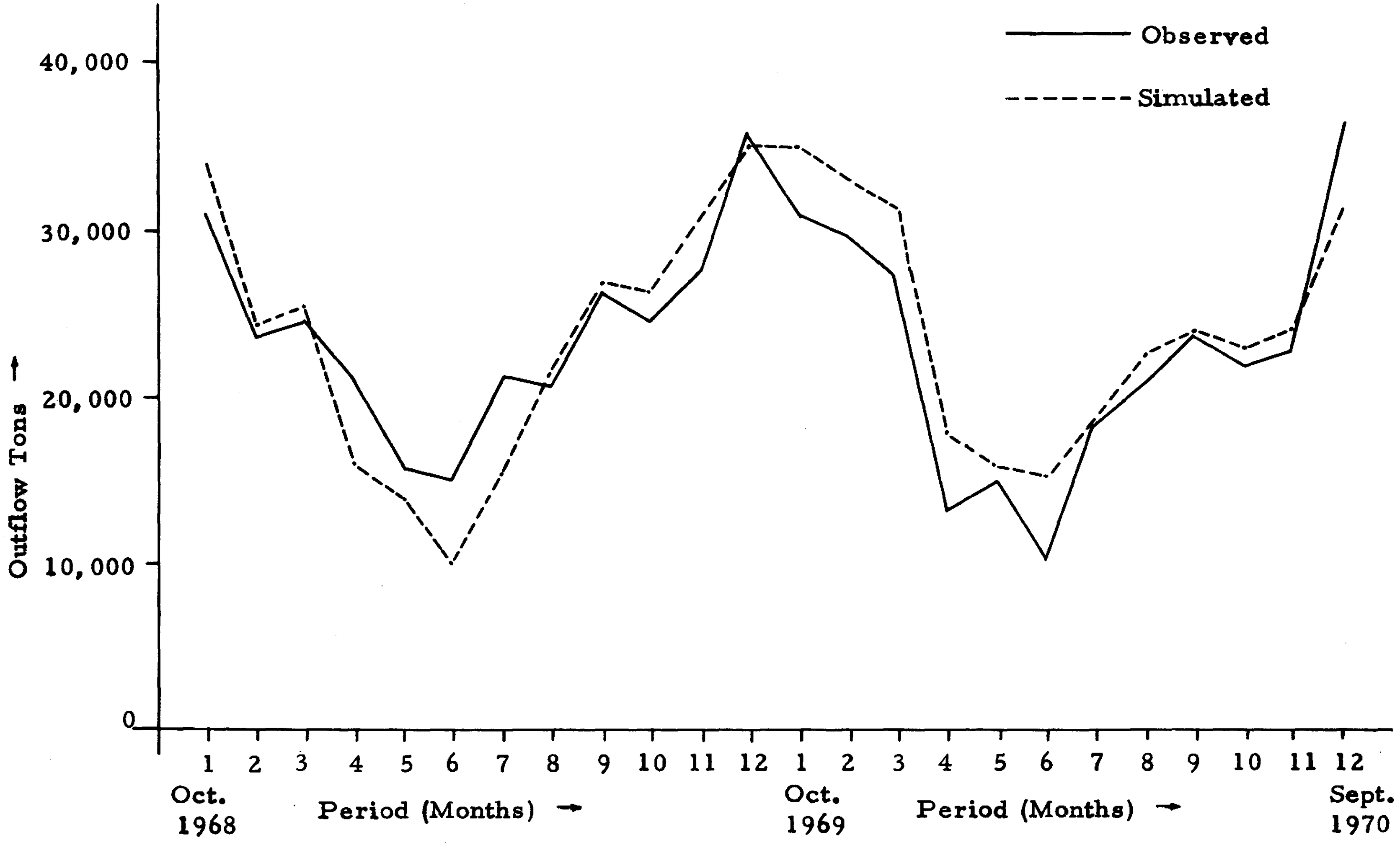

Figure 30. Observed and simulated TDS outflow.

predicted concentration of NO_3^- in the top layer of the soil profile is shown by Figure 31. It is seen that the average concentrations of NO_3^- in the top layer with the application of urea alone is much less com pared to the application of the combination of urea and ammonium type fertilizers. This is probably due to rapid hydrolysis of urea in the absence of any rate inhibiting compounds. The final quantity outflow of NO_3^- in the runoff water did not, however, show any appreciable difference, probably due to sufficient uptake of this nutrient by the growing crops.

Effects of land application of a typical effluent from an oxidation pond: In order to demonstrate the effects of this management situation, the characteristics of a typical effluent have been assumed to correspond to the analysis indicated by Environmental Protection Agency (1973) and shown by Table 10. Application of the existing source of irrigation water and also the fertilizer application have not been assumed in this study. Shown by Figure 32, is a typical distribution of the predicted concentration of NO_3^- in the top layer of the soil profile for the assumed management situation. It is seen from Figure 32 that the concentrations of NO_3^- are much in excess to the corresponding values under the existing management practice (Figure 31), namely application of irrigation water and fertilizers. The predicted quantities of NO_3^- and the total dissolved solids (TDS) in the runoff water are shown by Figure 33 and Figure 34, respectively. The predicted

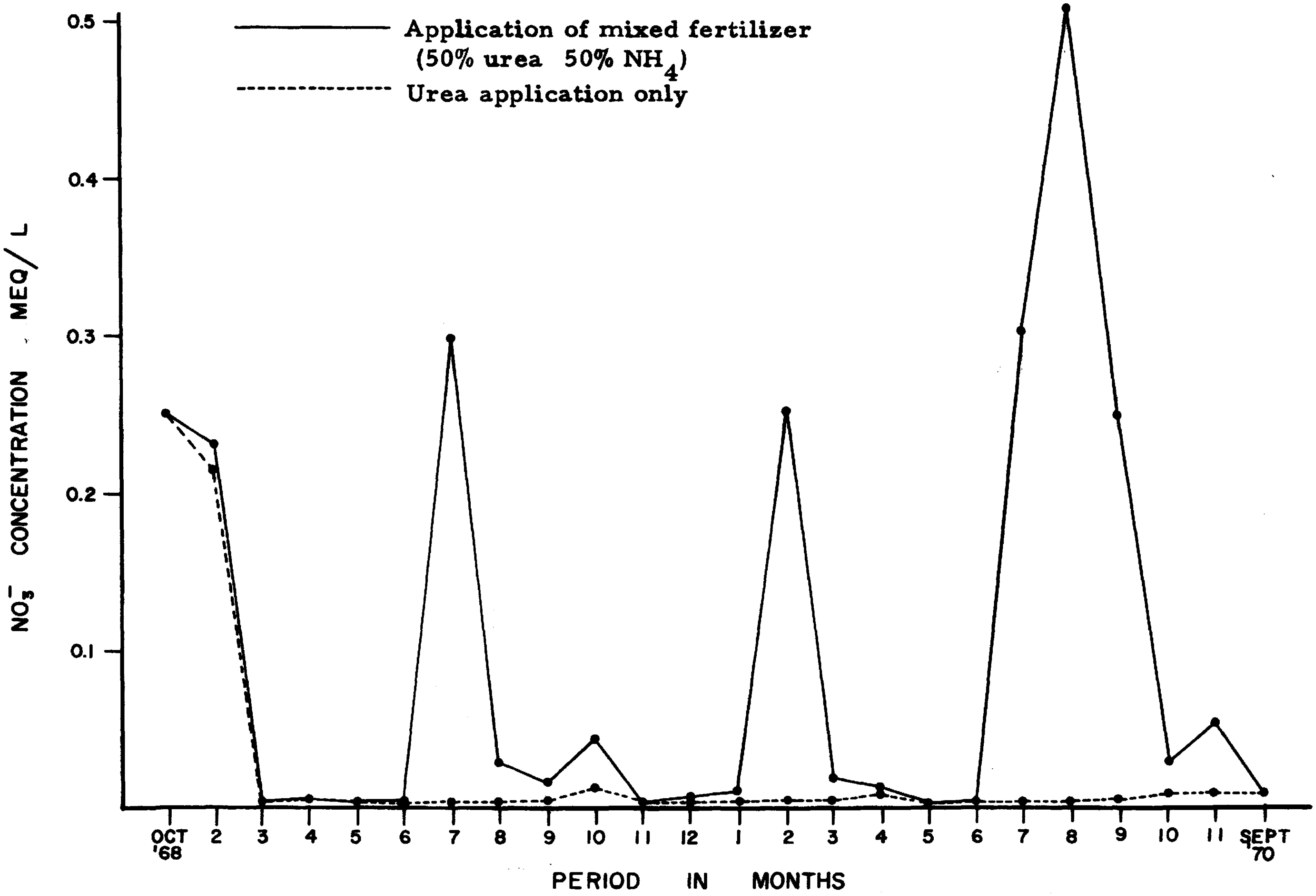

Figure 31. Predicted NO_3^- concentration in root zone (top layer) with different fertilizer applications.

Table 10. Typical characteristics of effluent from an oxidation pond.

Constituent	Concentration Mg/l
Chemical	
Specific conductivity, μmhos/cm	1140
Total dissolved solids	780
pH, units	7.3
BOD	15
Total nitrogen	25.2
Nitrate-nitrogen	14.2
Ammonia-nitrogen	6.1
Total phosphorus	13.0
Chlorides	158
Sulfate	115
Alkalinity ($CaCO_3$)	305
Boron	0.3
Sodium	150
Potassium	13
Calcium	30
Magnesium	49
Sodium adsorption ratio	3.9

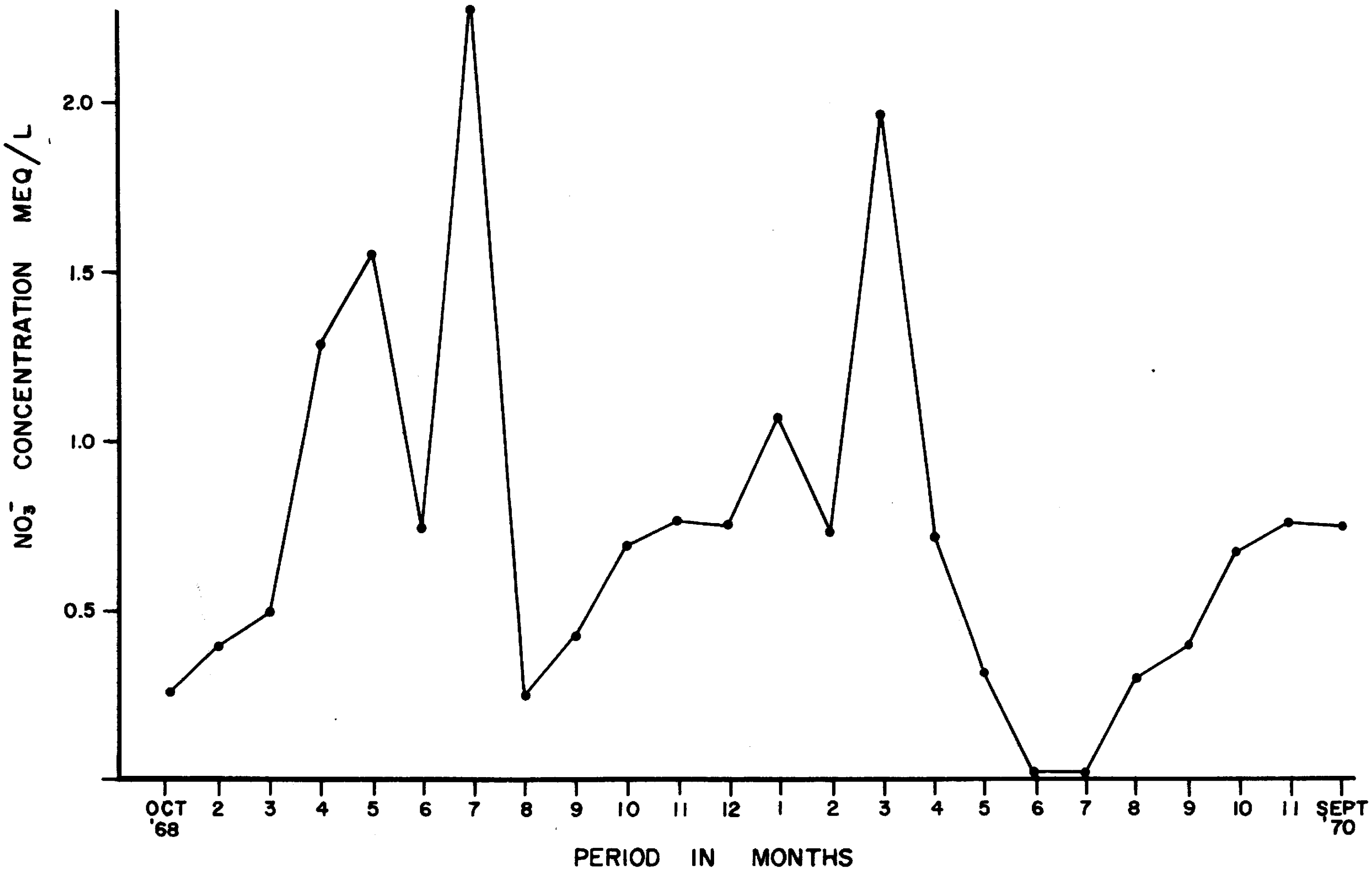

Figure 32. NO_3^- concentration in root zone (top layer) assuming application of typical effluent from oxidation pond.

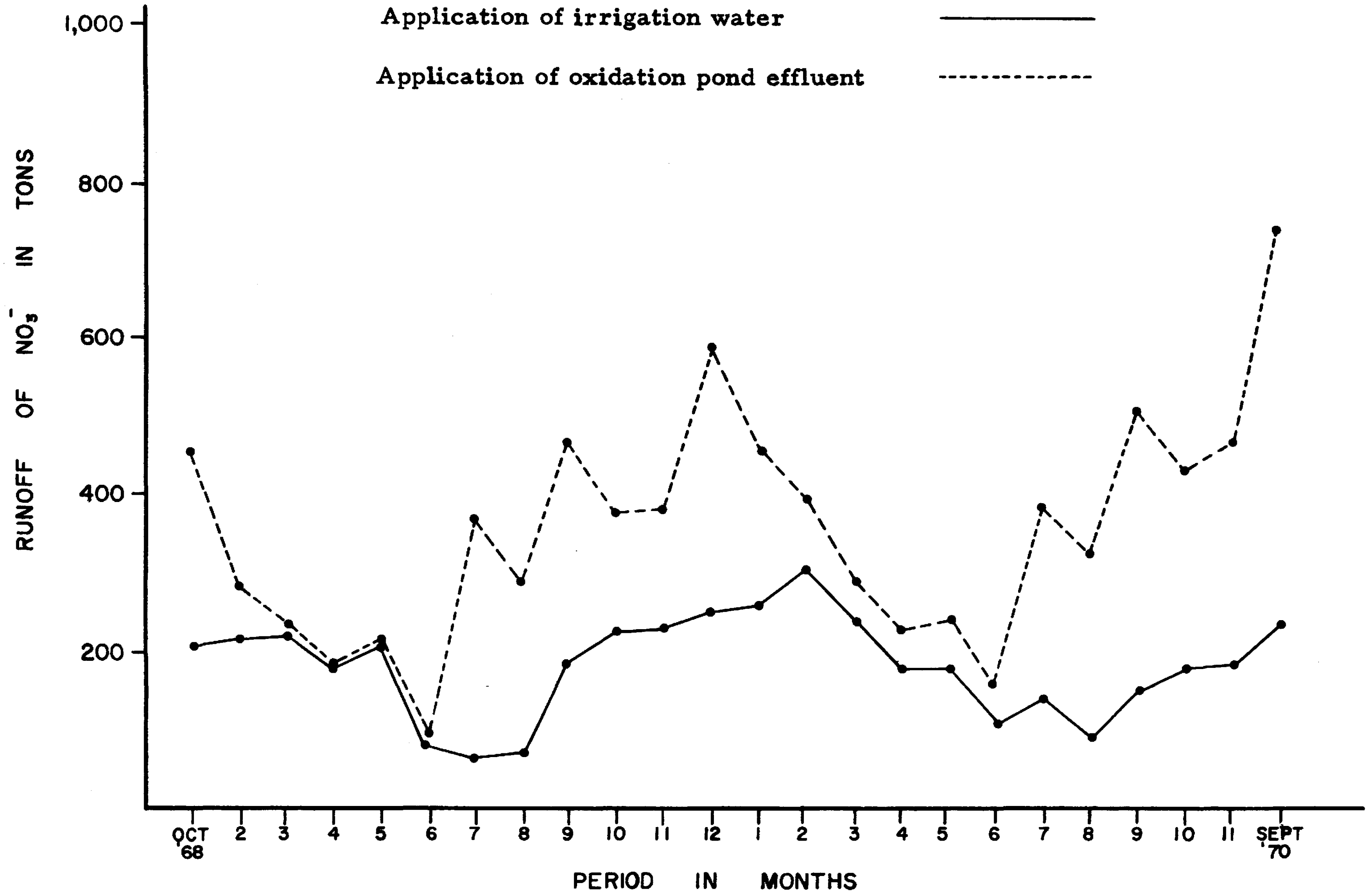

Figure 33. Effect of assumed application of oxidation pond effluent on the runoff of NO_3^-.

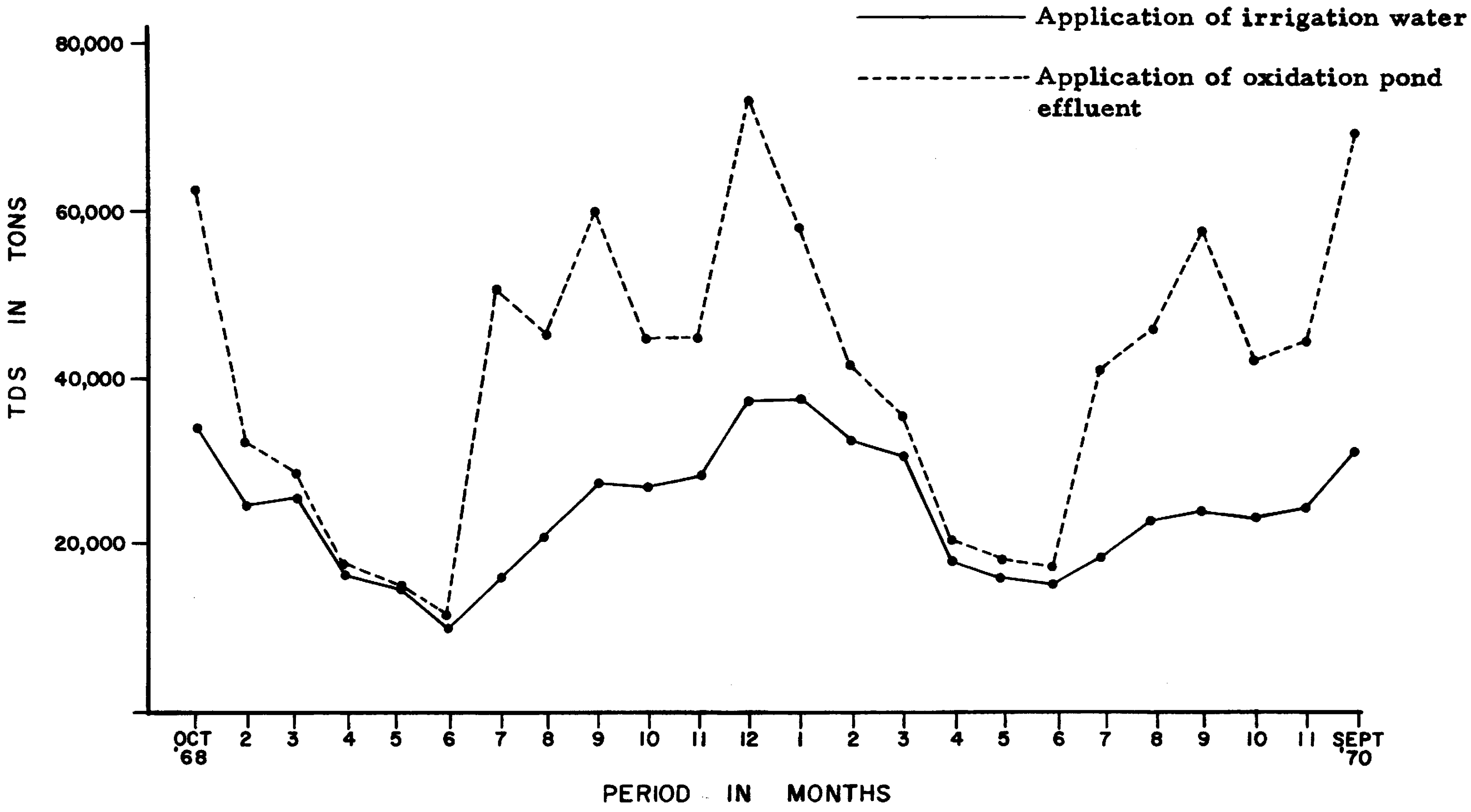

Figure 34. Effect of assumed application of oxidation pond effluent on the runoff of total dissolved solids (TDS).

quantities of NO_3^- shown in Figure 33, however, did not consider the nitrification in the overland flow, a feature not included in this model. The predicted quantity of TDS is about 74 percent in excess compared to the quantity with the existing management practice. The results appear to be in order as the average TDS of effluent from lagoon is about 780 ppm, while the TDS of the irrigation water is about 350 ppm. A similar increase has been noticed in respect to the remaining ions constituting the effluent salts.

Conclusions

The management studies indicated the usefulness of the model in predicting the effects of such changes in the basin on the effluent water quality. The sensitivity of the biological and chemical models in predicting the concentrations of NO_3^- within the root zone is also demonstrated by the management studies.

CHAPTER VII

SUMMARY AND CONCLUSIONS

Summary

A computer program was developed which combined the effects of biological changes on the chemical quality of water percolated through a soil profile, with a hydrologic model of an irrigated area of a river basin where subsurface runoff is predominant. The model was based on the work of Dutt et al. (1972) which incorporated improvements in chemical model and introduced a biological transformations model in respect to microbial nitrogen transformations within a soil profile. The combined model developed in this study is a significant improvement over the work of Thomas et al. (1971) in developing a comprehensive water quality model. The composite model operates the hydrology portion on a hybrid computer while the quality model is entirely digital. A variable spatial resolution and monthly time increment have been adopted to simulate the outflow of water and specific ions comprising the salt from an area in which irrigated agriculture is the predominant user of water. The seven individual ions considered in this study were calcium (Ca^{++}), Magnesium (Mg^{++}), sodium (Na^{+}), bicarbonate (HCO_3^-), chloride (Cl^-), nitrate (NO_3^-), and sulphate ($SO_4^=$).

The model was verified on the Snake River Plains, Twin Falls, Idaho, and it successfully predicted the quantities of water and the seven ions. All the predicted quantities of ions agreed within 10 percent on a weight basis, except sulphate ion, which comprises approximately 14 percent of total salts, showed significant variations for a few months in the calibration period. The correlation coefficients for the other ions for the two year model period, are within a range of 0.78 - 0.90. The sodium ion showed a closer fit in this study com pared to the results of Thomas et al. (1971). The results of nitrate ion are reasonably good.

The hydrology model which presently uses the hybrid computer can be entirely digital to make the composite model an all-digital program. The present program utilizes almost all the memory available on the 32,000 word digital computer. The program can handle two years of data with five different soils in each basin with 15 layers for each soil. Therefore, for longer periods of record or for other water quality parameters it would be necessary to adopt a computer with higher capabilities in addition to making the program entirely digital, as required.

Applicability of the Model

The hydro-quality model developed in this study is general in nature and has a variety of practical field applications. Some of the typical problems for which the model is useful are given as follows:

1. An examination of the effects of various management alternatives upon water quality (salinity) levels under

conditions of both present and projected land use patterns.

2. Studies involving the impacts of the quality of irrigation return flows upon downstream users.
3. Nitrate pollution of groundwaters.
4. Predictions of the quality of downstream waters when municipal sewage effluent is used for irrigation purposes.
5. Studies involving fertilizer management practices to predict the nitrogen uptake by crops while minimizing leaching losses to the groundwater.

Suggestions for Further Research

Invariably, all the research works lead to ideas and problems to be resolved. The research work reported herein is an attempt in terms of developing a comprehensive hydro-quality model. Further work is necessary for completing this goal as detailed below.

1. Improve the present model by making it an all-digital program to reduce both the memory required and also the operating time of the computer.
2. Test the model on areas where
    a. the source of water is municipal sewage effluent to demonstrate the prediction of the individual ions, and
    b. the nitrate ion constitutes a significant quantity of runoff.

3. Improve the nitrogen transformation model to reduce the number of assumptions made in this study and also to include the following:
    a. Study other types of equations with respect to rate of nitrogen transformations suitable for a gross monthly model.
    b. Develop rate equations for nitrogen transformations on the overland flow to represent adequately the rate of nitrification and uptake by aquatic biomass. This will facilitate applicability of the model where there is significant surface runoff compared to subsurface runoff. It will also adequately describe the nitrification process of a sewage effluent on land application.
    c. Include a temperature simulation model of the soil layers to adequately describe the temperature changes which affect the nitrogen transformations.
    d. Include a pathway of denitrification at the junction of soil water and groundwater table, a possibility that can occur in some of the areas.
4. Include the effects of other ions, namely the $PO_4^=$ and K^+, and $CO_3^=$.

5. Include the effects of other users, such as municipal and industrial, on the water quality parameters in the system.
6. Include other water quality parameters such as dissolved oxygen, temperature, biochemical oxygen demand, pesticides, radioactive elements, heavy metals, and coliforms.

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APPENDICES

APPENDIX A

Appendix A

Theoretical development of equations in chemical model

A. The mathematical relationships for the various chemical reactions considered in the chemical quality subsystem.

1. Solubility and precipitation of gypsum

Gypsum is a slightly soluble salt which is often present in the soil, added as a soil ammendment or formed when the solubility product is exceeded. The equation describing the relationship of gypsum with other constituents is

$$CaSO_4 \cdot 2H_2O \rightleftarrows Ca^{++} + SO_4^{=} + 2H_2O \quad . \quad . \qquad (A-1)$$

The solubility product $Ksp = \dfrac{A_{Ca}\, A_{SO_4}\, A^2_{H_2O}}{A_{CaSO_4} \cdot 2H_2O} = 2.4 \times 10^{-5}$

Assuming that activities of $CaSO_4 \cdot 2H_2O$ and H_2O are unity,

$$Ksp = C_{Ca}\, C_{SO_4}\, \gamma_{Ca}\, \gamma_{SO_4} \quad . \quad . \quad . \quad . \quad . \quad . \qquad (A-2)$$

Let M^o_{Ca} and $M^o_{SO_4}$ be initial molar concentrations of undissolved Ca^{++} and $SO_4^{=}$.

Let x be the amount that dissolves into gypsum. Then the final concentrations will be

$$M_{Ca} = M^o_{Ca} + x \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (A-3)$$

$$M_{SO_4} = M^o_{SO_4} + x \quad . \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (A-4)$$

Substituting in Equation (A-2) we get

$$Ksp = (M^o_{ca} + x)(M^o_{SO_4} + x)\,\gamma_{ca}\,\gamma_{SO_4} \qquad \text{(A-5)}$$

Assuming $\gamma_{ca} = \gamma_{SO_4} = \gamma$ and rearranging the terms Equation (A-5) can be written in the quadratic form

$$AX^2 + Bx + C = 0 \; . \; . \; . \; . \; . \; . \; . \; . \qquad \text{(A-6)}$$

in which

$A = 1$

$B = M^o_{ca} + M^o_{SO_4}$

$C = M^o_{ca}\ M^o_{SO_4} - Ksp/\gamma^2$

The Equation (A-6) is solved for X, the change in concentration of Ca^{++} and $SO_4^=$ to reach equilibrium.

2. Undissociated $CaSO_4$

The dissociation constant K_D of the ion pair $CaSO_4$ can be expressed as

$$K_D = \frac{M_{Ca} \cdot M_{SO_4} \cdot \gamma_{Ca}\,\gamma_{SO_4}}{M_{CaSO_4^o}\ \gamma_{CaSO_4^o}} \; . \; . \; . \; . \; . \qquad \text{(A-7)}$$

in which $K_D = 4.9 \times 10^{-3}$

$\gamma_{CaSO_4^o} = 1$

$M_{Ca} = M^o_{Ca} - Y$

$M_{SO_4} = M^o_{SO_4} - Y$

$M_{CaSO_4} = M^o_{CaSO_4} + Y$

and Y is the quantity of $CaSO_4$ formed. The Equation (A-7) can therefore be written in the form of a quadratic as

$$AY^2 + BY X C = 0 \quad . \quad . \quad . \quad . \quad . \quad . \quad . \qquad (A\text{-}8)$$

in which

$$A = \gamma^2$$

$$B = - [(M^o_{Ca} M^o_{SO_4}) \gamma^2 + K_D \gamma_{CaSO^o_4}] \qquad (A\text{-}9)$$

$$C = [M^o_{Ca} M^o_{SO_4} \gamma^2 - K_D \gamma_{CaSO^o_4} M^o_{CaSO_4}] \qquad (A\text{-}10)$$

Solving for Y we get the amount of $CaSO_4$ formed and precipitated.

3. Undissociated $MgSO_4$

The chemistry of undissociated $MgSO_4$ is similar to that of $CaSO_4$ and the equations are similar with appropriate dissociation constant of 6.3×10^{-3} for $MgSO_4$.

4. Dissolution or precipitation of lime

Lime is the least soluble salt in pure water without CO_2, with a solubility of about 14.3 mg/l for calcite and 15.3 mg/l for aragonite (Bathhurst, 1971) in the pressure-temperature range of surface waters. With the addition of CO_2 to the water, solubilities can reach hundreds of mg/l. The solubility product increases with increase in partial pressure of CO_2 and decreasing temperature.

The various equations describing the equilibrium of Carbonate waters are:

$$[Ca^{++}]\,[CO_3^{=}] = K_{CaCO_3} = 10^{-8.3} = Ksp \qquad (A\text{-}11)$$

$$\frac{[H^+]\,[HCO_3]}{[H_2CO_3]} = K_{H_2CO_3} = 10^{-6.4} = K_1 \qquad (A\text{-}12)$$

$$\frac{[H^+]\,[CO_3^{=}]}{[HCO_3]} = K_{HCO_3^-} = 10^{-10.3} = K_2 \qquad (A\text{-}13)$$

$$[H^+]\,[OH^-] = K_{H_2O} = 10^{-14} \qquad (A\text{-}14)$$

$$H_2CO_3 = P_{CO_2} \cdot K_{CO_2} \qquad (A\text{-}15)$$

Since $CO_3^{=}$ is a function of partial pressure of CO_2 and HCO_3^- concentration is usually the predominant form in which CO_2 occurs in soilwater system, it is more convenient to consider the following reaction.

$$H_2CO_3 + CaCO_3 \rightleftarrows Ca^{++} + 2HCO_3^-$$

$$K = \frac{[Ca^{++}]\,[HCO_3^-]^2}{[H_2CO_3]\,[CaCO_3]} \qquad (A\text{-}16)$$

$$= K_{sp} \cdot \frac{K_1}{K_2}$$

in which K_{sp}, K_1 and K_2 are defined in Equations (A-11), (A-12), and (A-13), respectively.

Assuming constant pressure of CO_2 and the activity coefficient of H_2CO_3 to be unity, the Equation (A-16) can be written as

$$Z = K\, C_{H_2CO_3} = [Ca^{++}]\,[HCO_3^-]^2$$

$$= M_{Ca} \cdot M_{HCO_3}^{\ 2} \cdot \gamma_{Ca}\, \gamma^2_{\ HCO_3} \qquad \text{(A-17)}$$

$$\text{and} \quad ZE = \frac{Z}{\gamma_{Ca}\, \gamma_{HCO_3}^{\ 2}} = M_{Ca}\, M_{HCO_3}^{\ 2} \qquad \text{(A-18)}$$

in which **M** is concentration and γ is the activity of associate ion. No attempt has been made in this study to incorporate the changes in solubility of $CaCO_3$ in the soil and also variation of H_2CO_3 content with soil moisture.

If x is the change in moles to reach equilibria, then

$$M_{Ca} = M^o_{\ Ca} + x \qquad \text{(A-19)}$$

$$M_{HCO_3} = M^o_{\ HCO_3} + 2\,x \qquad \text{(A-20)}$$

The Equation (A-18) will therefore be

$$ZE = (M^o_{\ Ca} + x)\,(M^o_{\ HCO_3} + 2\,x)^2 \qquad \text{(A-21)}$$

This can be written in the form

$$A\,x^3 + B\,x^2 + C\,x + D = 0 \qquad \text{(A-22)}$$

in which $A = 4$

$$B = 4\,[M^o_{\ Ca} + M^o_{\ HCO_3}]$$

$$C = [M^o_{\ HCO_3}{}^2 + 4\,M^o_{\ Ca} \cdot M^o_{\ HCO_3}]$$

$$D = [M^o_{\ HCO_3} \cdot M^o_{\ Ca} - ZE]$$

The Equations (A-19), (A-20), and (A-22) are used to compute the equilibrium concentrations of Ca^{++} and HCO_3^-.

5. Cation exchange reactions

The cation exchange reactions considered in the model are the Ca - Mg and Ca - Na reactions.

Ca - Mg exchange: An equation which has been extensively used to describe the exchange of Ca^{++} and Mg^{++} in soils is represented by

$$\begin{bmatrix}\text{Ratio of Cationic} \\ \text{species in the ex-} \\ \text{ternal equilibrium} \\ \text{solution}\end{bmatrix} = \begin{bmatrix}\text{Equilibrium} \\ \text{Constant}\end{bmatrix} \begin{bmatrix}\text{Ratio of equilibrium} \\ \text{Concentration of the} \\ \text{absorbed cationic} \\ \text{species}\end{bmatrix}$$

or

$$\frac{M_{Ca}}{M_{Mg}} = K \frac{M'_{Ca}}{M'_{Mg}} \qquad \text{(A-23)}$$

Let Y be the number of moles of Mg^{++} per gram of soil entering an exchange complex when a solution is brought into contact with soil colloids. Assuming that sum of exchangeable Ca^{++} and Mg^{++} is constant, the initial concentration of Ca^{++} and Mg^{++} is b_{Ca} and b_{Mg} moles per liter in the solution, and B_{Ca} and B_{Mg} moles per gram of soil in the soil exchange complex. Then

$$M'_{Ca} = B_{Ca} - Y \qquad \text{(A-24)}$$

$$M'_{Mg} = B_{Mg} + Y \qquad \text{(A-25)}$$

$$M_{Ca} = b_{Ca} + \beta Y \qquad \text{(A-26)}$$

$$M_{Mg} = b_{Mg} - \beta Y \qquad \text{(A-27)}$$

in which $\beta = \dfrac{\text{grams of oven dry soil}}{\text{liters of solution}} = 2000$, assumed in this study.

Combining all the above expressions with Equation (A-23) we get

$$\frac{b_{Ca} + \beta Y}{b_{Mg} - \beta Y} = K \, \frac{B_{Ca} - Y}{B_{Mg} + Y} \qquad \text{(A-28)}$$

Upon rearrangement we have:

$$\beta\,(1 - K)\,Y^2 + [\beta\,(B_{Mg} + KB_{Ca}) + b_{Ca} + Kb_{Mg}]\,Y$$
$$+ b_{Ca}\,B_{Mg} - K\,b_{Mg}\,B_{Ca} = 0 \qquad \text{(A-29)}$$

which is of the form $AY^2 + BY + C = 0$ (A-30)

The equation (A-30) is solved for Y to represent the changes in concentration of Ca^{++} and Mg^{++} to reach equilibrium in the solution complex.

Ca - Na exchange: Gapon equation used for Ca-Na exchange is

$$\frac{N_{Na}}{N_{Ca}} = K \, \frac{A_{Na}}{\sqrt{A_{Ca}}} \qquad \text{(A-31)}$$

in which

A denotes the activity of the ions indicated by the species,

K is the exchange constant, and

N denotes the concentration of exchangeable ions indicated by the species.

Let y moles of Ca^{++} per gm of soil that go into solution;

b_{Ca}, b_{Na} are moles/liter of Ca^{++} and Na^{+} in solution phase.

B_{Ca}, B_{Na} moles/gm adsorbed on the soil exchange complex.

Therefore, the relative change in composition of solution and adsorbed phases are:

$$N_{Ca} = B_{Ca} - y \tag{A-32}$$

and $N_{Na} = B_{Na} + 2y$ in the adsorbed phase (A-33)

$$C_{Ca} = b_{Ca} + \beta y \tag{A-34}$$

and $C_{Na} = b_{Na} - 2\beta y$, in the solution phase, in which β is already defined.

Substituting the values for N_{Ca}, N_{Na}, C_{Ca}, and C_{Na} in Equation (A-31),

$$\frac{N_{Na}}{N_{Ca}} = K \frac{\gamma_{Na} C_{Na}}{\sqrt{\gamma_{Ca} C_{Ca}}}$$

or

$$\frac{B_{Na} + 2y}{B_{Ca} - y} = K \frac{\gamma_{Na} (b_{Na} - 2\beta y)}{\sqrt{\gamma_{Ca} (b_{Ca} + \beta y)}} \tag{A-36}$$

For a uniform ionic strength $\gamma_{Ca} = \gamma_{Na}^{4}$. Denoting $\gamma = \frac{\gamma_{Ca}}{\gamma_{Na}}$, the Equation (A-36) can be written:

$$Ay^4 + By^3 + Cy^2 + Dy + E = 0 \tag{A-37}$$

in which,

$$A = -4K^2\beta^2$$

$$B = 4\beta(\gamma^{1/2} + K^2 b_{Na} + 2K^2 B_{Ca}\beta)$$

$$C = 4\gamma^{1/2}(b_{Ca} + \beta B_{Na}) - 4K^2 B_{Ca}\beta(B_{Ca}\beta + 2b_{Na}) - K^2 b_{Na}^2$$

$$D = \gamma^{1/2} B_{Na}(4b_{Ca} + \beta B_{Na}) + 2K^2 b_{Na} B_{Ca}(2B_{Ca}\beta + b_{Na})$$

and

$$E = \gamma^{1/2} B_{Na}^2 b_{Ca} - K^2 b_{Na}^2 B_{Ca}^2$$

The Equation (A-37) is solved for y, the change in concentration required to reach equilibrium from initial or approximate conditions.

B. Mathematical relationship for the equilibrium concentrations of ions in solution and on exchange complex, used in subroutine EQEXCH

1. Equilibrium concentrations of ions in solution

Considering the formation of ion pairs, the total equilibrium concentration of the ions Ca^{++}, Mg^{++} and $SO_4^=$ are given by:

$$C_{Ca_t} = C_{Ca} + C_{CaSO_4} \qquad \text{(A-38)}$$

$$C_{Mg_t} = C_{Mg} + C_{MgSO_4} \qquad \text{(A-39)}$$

$$C_{SO_{4_t}} = C_{SO_4} + C_{CaSO_4} + C_{MgSO_4} \qquad \text{(A-40)}$$

The thermodynamic equilibrium constant, K, for equilibrium between the undissociated species in solution and the appropriate ions would be

$$K_{CaSO_4} = \frac{A_{Ca}\, A_{SO4}}{A_{CaSO_4}}\,, \quad K_{MgSO_4} = \frac{A_{Mg}\, A_{SO4}}{A_{MgSO_4}} \quad . \; . \; . \; . \; . \; . \quad \text{(A-41, A-42)}$$

Combining the Equations (A-41)and (A-38)

$$C_{CaSO_4} = \frac{\gamma_{SO_4}\, \gamma_{Ca}\, C_{Ca_t}\, C_{SO_4}}{K_{CaSO_4} + \gamma_{Ca}\, \gamma_{SO_4}\, C_{SO_4}} \qquad \text{(A-43)}$$

and similarly combining Equations (A-42) and (A-39)

$$C_{MgSO_4} = \frac{\gamma_{SO_4}\, \gamma_{Mg}\, C_{Mg_t}\, C_{SO_4}}{K_{MgSO_4} + \gamma_{Mg}\, \gamma_{SO_4}\, C_{SO_4}} \qquad \text{(A-44)}$$

Assume that divalent activity coefficients are equal, namely

$$\gamma_{Ca} = \gamma_{SO_4} = \gamma_{Mg} = \gamma_2$$

Combining Equations (A-40, 43, and 44) it is found that:

$$Ax^3 + Bx^2 + Cx + D = 0 \qquad \text{(A-45)}$$

in which

$$A = {\gamma_2}^2$$

$$B = \gamma_2 [(K_{CaSO_4} + K_{MgSO_4}) + \gamma_2 (C_{Mg_t} + C_{Ca_t} - C_{SO_{4_t}})]$$

$$C = K_{CaSO_4}\, K_{MgSO_4} + \gamma_2 [C_{Mg_t}\, K_{CaSO_4} + Ca_t\, K_{MgSO4} - C_{SO_{4_t}} (K_{CaSO_4} + K_{MgSO_4})]$$

$$D = -\, C_{SO_{4_t}}\, K_{MgSO_4}\, K_{CaSO_4}$$

Equation (A-45) is solved for x, the equilibrium concentrations of $SO_4^{=}$ ion. The equilibrium concentrations of Ca and Mg ions are obtained from Equations (A-39) and (A-40).

2. Concentration of exchangeable cations

Total concentration of exchangeable cations is given by:

$$N_t = N_{Na} + N_{Ca} + N_{Mg} \qquad \text{(A-46)}$$

in which N denotes the concentrations of ion indicated by the subscript.

Ca - Mg exchange is described by

$$\frac{A_{Ca}}{A_{Mg}} = K_1 \frac{N_{Ca}}{N_{Mg}} \qquad \text{(A-47)}$$

and, Ca - Na exchange is described by

$$\frac{A_{Na}}{\sqrt{A_{Ca}}} = K_2 \frac{N_{Na}}{N_{Ca}} \qquad \text{(A-48)}$$

Combining Equations (A-46), (A-47), (A-48) :

$$N_t = \frac{A_{Na}}{\sqrt{A_{Ca}}} \cdot \frac{N_{Ca}}{K_2} + K_1 \frac{N_{Ca} \cdot A_{Mg}}{A_{Ca}} + N_{Ca}$$

$$= N_{Ca} \left[\frac{A_{Na}}{K_2 \sqrt{A_{Ca}}} + K_1 \frac{A_{Mg}}{A_{Ca}} + 1 \right]$$

or

$$N_{Ca} = N_t \Big/ \left[\frac{A_{Na}}{K_2 \sqrt{A_{Ca}}} + K_1 \frac{A_{Mg}}{A_{Ca}} + 1 \right] \qquad \text{(A-49)}$$

Knowing the activity coefficients, the ionic concentrations for an equilibrium soil extract for Ca, Mg, Na, and the total exchangeable bases, the exchangeable Ca can be calculated from Equation (A-49). Exchangeable Na and Mg are calculated from Equations (A-48) and (A-46) respectively.

APPENDIX B

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C     A HYDRO-QUALITY MODEL TO PREDICT THE EFFECTS OF BIOLOGICAL
C     TRANSFORMATIONS ON THE CHEMICAL QUALITY OF RETURNFLOW
C     OPTIMAL VERIFICATION BY MODIFIED PATTERN SEARCH METHOD-OPVER
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BO,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      COMMON/BLK3/PCA(24,5),PCL(24,5),PHCO3(24,5),PMG(24,5),PNA(24,5),
     1PNO3(24,5),PSO4(24,5),OBJ,CCA(70),CMG(70),CNA(70),CCL(70),
     2CHCO3(70),CSO4(70),CCNO3(70)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
     1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
     2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
     3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
     4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
      DIMENSION PT(16)
      DATA PT(1),PT(2),PT(3),PT(4),PT(5),PT(6),PT(7),PT(8),PT(9),PT(10),
     1PT(11),PT(12),PT(13),PT(14),PT(15),PT(16)
     2    /4HP010,4HP011,4HP012,4HP013,4HP014,4HP015,4HP016,4HP017,
     34HP018,4HP019,4HP020,4HP021,4HP022,4HP023,4HP024,4HP025/
C
      CALL QSHYIN(IERR,500)
      CALL QSC(1,IERR)
      PAUSE 1
      CALL QSSECN(IERR)
      CALL QSDLY(10)
    1 READ (6,100) ITY
      IF(ITY) 99,99,2
C     ITY=0 GO TO QUALITY SUBROUTINE
    2 GO TO (5,9,10,1000),ITY
C     ITY=1 OPERATE AS ORIGINAL PROGRAM RETURN AFTER 230 IN HYDSM
C     ITY=2 OPTIMAL VERIFICATION ONLY
C     ITY=3 PLOT OBSERVED OUTFLOW AND COMPUTED OUTFLOW
C     ITY=4 PROGRAM STOPS
    5 IENT=1
      IRET=0
      GO TO 80
C     READ NUMBER OF PHASES(NPH) AND NUMBER OF PARAMETERS
    9 READ(6,100) NPH,NPR
      DO309 LL=1,NPR
  309 READ(6,301) L,XIN(1,L),PL(L),PM(L),NL(L)
  310 OBI(1)=OBJ
C     INITIALIZE MINIMUM CONDITIONS
      PRMN=OBJ
      PHMN=OBJ
      DO 314 L=1,NPR
      XMN(L)=XIN(1,L)
      XPM(L)=XIN(1,L)
      PR(L)=XIN(1,L)
  314 DF(L)=PM(L)-PL(L)
C     TAKE A NEW PAGE WRITE PM,PL,NL
      WRITE(6,302)
      DO 315 L=1,NPR
  315 WRITE(6,303) L,PM(L),PL(L),DF(L),NL(L)
C     BEGIN PHASE LOOP
      DO 390 K=1,NPH
C     TAKE NEW PAGE WRITE PHASE ONE INITIAL VECTOR
      WRITE(6,304) K,PHMN
      WRITE(6,305)(XIN(K,L),L=1,NPR)
      WRITE(6,306)
C     BEGIN PAR LOOP
      DO 380 J=1,NPR
      NLO=NL(J)+1
C     NO OF LEVELS =NLO
      IF(NLO.LE.2) GO TO 380
C     BEGIN INCREMENT LOOP
      DO 370 IK=1,NLO
      IF(IK.GT.1) GO TO 340
      XNL=NL(J)
      DS=DF(J)/XNL
  340 XI=(IK-1)
C     INCREMENTED LEVEL
      PR(J)=PL(J)+DS*XI
C     OPERATE MODEL AND DETERMINE OBJ
  349 CALL PARSET(J,PR(J))
      CALL HYDSM(2,2,OBJ)
      WRITE(6,307) J,IK,PR(J),OBJ
C     IF NEW PAR INITIALIZE LOCAL MIN
      IF(IK.GT.1)GO TO 367
      PRMN=OBJ
      XMN(J)=PR(J)
C     CHECK LOCAL AND PHASE MINS
      GO TO 351
  367 IF(OBJ-PRMN) 350,351,351
  350 PRMN=OBJ
      XMN(J)=PR(J)
  351 IF(OBJ-PHMN) 352,370,370
  352 PHMN=OBJ
      DO 353 L=1,NPR
  353 XPM(L)=PR(L)
  370 CONTINUE
C     RESET PR(J) TO FIXED LEVEL FOR NEXT PAR
  372 PR(J)=XMN(J)
      CALL PARSET(J,PR(J))
      CALL HYDSM(2,2,OBJ)
  380 CONTINUE
C     SELECT BEST VECTOR NEXT PHASE
      IF(PRMN-PHMN) 384,386,386
  384 KFJ=K+1
      DO 385 L=1,NPR
      XIN(KFJ,L)=XMN(L)
      PR(L)=XMN(L)
  385 CALL PARSET(L,PR(L))
      GO TO 388
  386 KFJ=K+1
      DO 387 L=1,NPR
      XIN(KFJ,L)=XPM(L)
      PR(L)=XPM(L)
  387 CALL PARSET (L,PR(L))
  388 CALL HYDSM(2,2,OBJ)
      OBI(K+1)=OBJ
  390 CONTINUE
C     WRITE OUT INITIAL VECTOR TABLE
      NHP=NPH+1
      WRITE(6,109) (OBI(L),L=1,NHP)
```

```
      WRITE(6,110)
      NPT=NPH+1
      DO 91 L=1,NPR
   91 WRITE(6,111)L,(XIN(M,L),M=1,NPT)
C     SET ALL PARAMETERS TO OPTIMAL VALUE AND OPERATE
      DO 228 L=1,NPR
  228 CALL PARSET(L,XIN(NHP,L))
      WRITE(6,105)
      CALL HYDSM(2,3,OBJ)
      GO TO 1
   80 CALL HYDSM(IENT,IRET,OBJ)
      GO TO 1
   10 CALL GRAPH
      GO TO 1
   99 CALL QUAL
      GO TO 1
  100 FORMAT(16I5)
  105 FORMAT(//46H I J QMES QSIM   DIF   QGR   SRF   SUBSF  GWBF,
     121HSNPC  STRC   DAL   DP///)
  109 FORMAT(1H1//27X,15HINITIAL VECTORS//10X5HPHASE,7X,1H1,9X,1H2,9X,
     11H3,9X,1H4,9X,1H5//12X,3HOBJ,5F10.4/)
  110 FORMAT(12X,3HPAR/)
  111 FORMAT(12X,I3,5F10.3)
  301 FORMAT(I2,3(F6.2,2X),I2)
  302 FORMAT(1H1///27X,3HPAR,8X,2HPM,8X,2HPL,8X,2HDF,8X,2HNL///)
  303 FORMAT(25X,I7,3X,3F10.3,I7)
  304 FORMAT(1H1//20X,5HPHASE,I3,2X,5HPMIN=,F10.4)
  305 FORMAT(5X,10F7.3)
  306 FORMAT(///6X,26HIP   LV     PAR        OBJ)
  307 FORMAT(5X,I3,2X,I3,F11.3,5F11.4)
  308 FORMAT(5X,I3,2H *,I3,F11.3,5F11.1)
 1000 STOP
      END

C     BASIC DATA FOR B-C ET-SUBROUTINE BASIC
      SUBROUTINE BASIC
      COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
     1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
     2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
     3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
     4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
      READ(5,100) LYRO,NYR
      READ(6,110) (VV(I),I=1,13)
      READ(6,115) (B(I),I=1,9)
C     READ PERCENT DAYLIGHT HOURS LAT42-30N
      READ(6,102) (PDL(K),K=1,12)
C     READ USE COEFFICIENTS
      DO52I=1,9
   52 READ(6,220)(WKC(I,J),J=1,12)
C     WRITE INITIAL DATA
      WRITE(6,110) (VV(I),I=1,13)
      WRITE(6,102)(PDL(K),K=1,12)
      WRITE(6,115) (B(I),I=1,9)
      DO 500I=1,9
  500 WRITE(6,221) I,B(I),(WKC(I,J),J=1,12)
  100 FORMAT(16I5)
  102 FORMAT(12F6.2)
  110 FORMAT(13(3XA3))
  115 FORMAT(9(3XA4))
  220 FORMAT(10X12F5.0)
  221 FORMAT(1X,I2,A7,12F5.0)
  230 RETURN
      END
```

```
C      SUBROUTINE FOR SYSTEM HYDROLOGY
       SUBROUTINE HYDSM(IENT,IRET,OBJ)
       COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
      1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
      2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
      3TXX(20),XLIME(20),XM,ZE(20)
       COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
      1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
      2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BH3(4),BC,D1,
      3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
      4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
      5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
      6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
       COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
      1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
      2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
       COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
      1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
      2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
      3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
      4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
       GO TO (8,9),IENT
     8 CALL BASIC
       CALL HYDDAT (IENT,IRET)
C
       DO 2 I=1,6
     2 DDA(I)=0.
       CALL QWBDAR(DDA,0,5,IERR)
       CALL QSTDA
C      INITIALIZE OBJECTIVE FUNCTION
     9 OBJ=0.
       OBA=0.
       ARF1=AGINIC
C      SET ANALOG TO INITIAL MODE
       CALL QSIC(IERR)
C      REPEAT PROCEDURE FOR EACH YEAR
       K=0
       SUMM=0.
       SUMC=0.
       YSUM=0.
       YSQR=0.
       I=0
       IF(IRET.EQ.0) WRITE(6,5)
       DO 225 II=1,NYR
       QMEASA=0.
       QSIMA=0.
C      REPEAT OPERATIONS FOR EACH MONTH
       DO 222 JJ=1,12
       I=I+1
       K=K+1
C      INITIALISE TEMP,PDH,XKC,PRE
       TEMP=DUM(II,JJ,7)
       PDH=PDL(JJ)/100.
       XKC=SWKC(JJ)/100.
       PRE=DUM(II,JJ,8)
C      COMPUTE SNOWMELT
       IF(TEMP.GT.32.) GO TO 606
C      SNO= INITIAL WATER EQUIVALENT OF SNOW PACK
       SNO=SNO+PRE
       PSM=0.
       GO TO 605
   605 WS=SNO*EXP(SMC*(TEMP-32.))
```

```
C      MONTHLY SNOWMELT=FNR
       FNR=SNO-WS
       SNO=WS
       PSM=PRE+FNR
  605  SP=PSM
C      SNOWMELT+PRECIP
       DDA(1)=SP/SKAL
C      COMPUTE ET BY BLANEY CRIDLE- INCHES
       E=XKC*(0.0173*TEMP-.314)*TEMP*PDH/SKAL
C      DIVERSIONS TO LAND- INCHES
       Q=(DUM(II,JJ,1)+DUM(II,JJ,6))*12./(AREA*SKAL)
C
       DDA(2)=-E
       DDA(3)=Q
C      INITIAL MOISTURE CONTENT=DIG(7)
       DDA(4)=DIG(7)/SKAL
       DDA(5)=DIG(2)/SKAL
C      IRRIGATION EFFICIENCY=EFF(JJ)
       DDA(6)=EFF(JJ)*DDA(3)
C      TRANSFER DATA FROM DIGITAL TO ANALOG
  600  CALL QWBDAR(DDA,00,6,IERR)
       CALL QSTDA
C      TEST SENSE LINE TO PROCEED COMPUTATIONS
  611  CALL QRLBB(ITEST,IERR)
       IF(ITEST.EQ.'200) GO TO 611
  612  CALL QRLBB(ITEST,IERR)
       IF(ITEST.NE.'200) GO TO 612
       CALL QSOP (IERR)
  613  CALL QRLBB(ITEST,IERR)
       IF(ITEST.EQ.'200) GO TO 613
       CALL QSH(IERR)
C      TRANSFER DATA FROM ANALOG TO DIGITAL
       CALL QRBADR(A8,0,9,IERR)
       DP(I)=SKAL*A8(1)
       EVT(I)=SKAL*A8(2)
       SM(I)=SKAL*A8(3)
       DAL(I)=SKAL*A8(4)
       SRF(I)=-SKAL*A8(5)
       SNPC(I)=A8(6)*SKAL*SPC
       STRC1(I)=-SKAL*A8(7)
       GWBF(I)=SKAL*A8(9)
       ARF2=A8(8)*SKAL
       ARF=(ARF1+ARF2)/2.
       SUBSRF(I)=ARF*FK(JJ)
C      COMPUTED OUTFLOW
       SUMOUT(I)=SRF(I)+SNPC(I)+STRC1(I)+SUBSRF(I)+GWBF(I)
       SIM(II,JJ)=SUMOUT(I)
C      COMPUTE MEASURED SURFACE RUNOFF - INCHES
       QMEAS=0.
       DO 150 MM=2,5
  150  QMEAS=DUM(II,JJ,MM)+QMEAS
       QMEASI=QMEAS*12./AREA
       OBS(II,JJ)=QMEASI
       QGOUT=SUMOUT(I)*AREA/12.
C      NET CHANGE IN SOIL MOISTURE
       SMCH(I)=FNR+PRE+DAL(I)-EVT(I)
C      COMPUTE BASE FLOW
       QGOUT=GWBF(I)+SUBSRF(I)
       ARF1=ARF2
C      CALCULATE OBJ
       DIFF=QMEASI-SUMOUT(I)
       QMEASA=QMEASA+QMEASI
       QSIMA=QSIMA+SUMOUT(I)
```

```
       IF(IRET.EQ.3) GO TO 250
       DIFF=ABS(DIFF)
       OBJ=OBJ+(DIFF)**2
       IF(IENT.EQ.2) GO TO 222
C
       WRITE(6,103) II,JJ,SRF(I),SUBSRF(I),EVT(I),GWBF(I),SNPC(I),
      1STRC1(I),SMCH(I),DAL(I),DP(I),SUMOUT(I),QMEASI,DIFF
       GO TO 222
  250  WRITE(6,103) II,JJ,QMEASI,SUMOUT(I),DIFF,QGOUT,SRF(I),SUBSRF(I),
      1GWBF(I),SNPC(I),STRC1(I),DAL(I),DP(I)
  222  CONTINUE
       IF(IRET.EQ.2) GO TO 225
       DIFFA=QMEASA-QSIMA
       IF(IRET.EQ.3) GO TO 251
       WRITE(6,104) QMEASA,QSIMA,DIFFA
  251  SUMM=SUMM+QMEASA
       SUMC=SUMC+QSIMA
  225  CONTINUE
       IF(IRET.EQ.2) GO TO 230
C      COMPUTE CORRELATION COEFFICIENT
       NMO=K
       XNO=NMO
       YSQR1=0.
       DX=0.
       DY=0.
       XBAR=SUMM/XNO
       YBAR=SUMC/XNO
       DO 15 II=1,NYR
       DO 15 JJ=1,12
       DIFFX=OBS(II,JJ)-XBAR
       DIFFY=SIM(II,JJ)-YBAR
       YSQR=DIFFX*DIFFY
       DIFFX=DIFFX*DIFFX
       DIFFY=DIFFY*DIFFY
       DX=DX+DIFFX
       DY=DY+DIFFY
   15  YSQR1=YSQR1+YSQR
       YSQR1=YSQR1*YSQR1
       DNR=DX*DY
       RR=YSQR1/DNR
       RRR=SQRT(RR)
       SUMM=SUMM*AREA/12.
       SUMC=SUMC*AREA/12.
       WRITE(6,105) RR,RRR,SUMM,SUMC
    5  FORMAT(54H YR MO SRF  SUBSRF EVT   GWBF  SNPC  STRC SMCH    DAL ,
      124H  DP  SUMOUT QMEAS DIFF )
  103  FORMAT(2I3,12F6.2)
  104  FORMAT(2X,3F8.3)
  105  FORMAT(//5H R*R=,F6.4,2X,2HR=,F6.4,2X,11HTOTAL MEAS=,F10.0,
      12X,11HTOTAL CALC=,F10.0)
  230  RETURN
       END
```

```
C     HYDROLOGIC DATA INPUT - SUBROUTINE HYDDAT
C     SUBROUTINE HYDDAT
      SUBROUTINE HYDDAT(IENT,IRET)
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DOA(6),DCA(9),DD(12),
     1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
     2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
     3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
     4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
      DIMENSION PT(16)
      DATA PT(1),PT(2),PT(3),PT(4),PT(5),PT(6),PT(7),PT(8),PT(9),PT(10),
     1PT(11),PT(12),PT(13),PT(14),PT(15),PT(16)
     2    /4HP010,4HP011,4HP012,4HP013,4HP014,4HP015,4HP016,4HP017,
     34HP018,4HP019,4HP020,4HP021,4HP022,4HP023,4HP024,4HP025/
      GO TO (101,102),IENT
C     INPUT CROP ACRAGES FOR BASIN
  101 DO 54 J=1,9
   54 CAC(J)=0.0
      READ(6,221)(I1(J),DCA(J),J=1,9)
      SCAC=0.0
      DO 55J=1,9
      L=I1(J)
      IF(L.LF.0) GO TO 55
      CAC(L)=DCA(J)
      SCAC=SCAC+CAC(L)
   55 CONTINUE
C     COMPUTE CROP PROPORTIONS
   57 DO 60 J=1,9
   60 PCP(J)=CAC(J)/SCAC
C     COMPUTE WEIGHTED USE COEFFICIENTS
      DO 70J=1,12
      SCKC=0.0
      DO69L=1,9
   69 SCKC=SCKC+WKC(L,J)*PCP(L)
   70 SWKC(J)=SCKC
      WRITE(6,222)(CAC(J),J=1,9),SCAC
      WRITE(6,223)(PCP(J),J=1,9)
      WRITE(6,224)(SWKC(J),J=1,12)
C     DIGITAL AND ANALOG PARAMETERS
      READ(6,104) (EFF(L),L=1,12)
      READ(6,104) (FK(L),L=1,12)
      READ(6,104)(DIG(L),L=1,10)
      READ(6,105)(PH(L),L=1,15)
      WRITE(6,104)(DIG(L),L=1,10)
      WRITF(6,105)(PH(L),L=1,15)
      WRITE(6,104) (EFF(L),L=1,12)
      WRITE(6,104) (FK(L),L=1,12)
      AREA=202700.
      CONV=12.0*43560.
      SKM=1000.
C     INITIALIZE DUM
      DO86II=1,NYR
      DO86JJ=1,12
      DO86J=1,8
   86 DUM(II,JJ,J)=0.
C     READ ALL INITIAL DATA IN ACREFT:TEMP IN F: PRECP-INCHES.
      DO99II=1,NYR
      DO99 J=1,8
      IF(J-7) 200,98,98
  200 IF(J-5) 202,202,203
  202 READ(6,201) (DD(JJ),JJ=1,12)
      GO TO 87
  203 READ(6,204) (DD(JJ),JJ=1,12)
      GO TO 95
   87 IF(J-5) 90,90,95
   90 DO 91 JJ=1,12
   91 DUM(II,JJ,J)=(DUM(II,JJ,J)+DD(JJ))*SKM
      GOTO 97
   95 DO 96 JJ=1,12
   96 DUM(II,JJ,J)=DUM(II,JJ,J)+DD(JJ)
   97 L=LYRO+II-1
      WRITE(6,230) J,L,(DUM(II,JJ,J),JJ=1,12)
      GO TO 99
   98 CALL PRETEM(L)
   99 CONTINUE
C     DIGITAL VALUES
  102 SNO=DIG(1)
      FMIN=DIG(3)
      FMES=DIG(2)
      SMC=DIG(4)
      SPC=DIG(5)
      SKAL=DIG(6)
      FMCS=DIG(3)
      AGINIC=DIG(8)
      TI=DIG(9)
   17 PH(4)=PH(4)/SKAL
      PH(5)=PH(5)/SKAL
      PH(15)=.1*PH(15)/SKAL
      DO 19 L=1,15
      CALL POTST (L,PH(L),PT)
   19 CONTINUE
   20 WRITE(6,303)
      WRITE(6,302)(PH(L),L=1,15)
      WRITE(6,301)
C     READ ANALOG COMPONENTS
      CALL QSPS(IERR)
      DO 5 L=1,15
      PADR=PT(L)
      CALL QRAR(PADR,PVAL,IERR)
    5 PVV(L)=PVAL
      WRITE(6,302)(PVV(L),L=1,15)
  104 FORMAT(12F6.2)
  105 FORMAT(12F6.2/12F6.2)
  201 FORMAT(12F6.1)
  204 FORMAT(12F6.0)
  221 FORMAT(10X,6(I3,F7.0)/10X,3(I3,F7.0))
  222 FORMAT(1X7F9.0/1X3F9.0)
  223 FORMAT(1X,7F9.5/1X,2F9.5)
  224 FORMAT(1X12F6.2)
  230 FORMAT(1XI2,I5,9F8.0/8X,3F8.0)
  301 FORMAT(35H POTS 10 THRU 24 ARE SET AS FOLLOWS)
  302 FORMAT(1X8F8.5)
  303 FORMAT(41H POTS 10 THRU 24 SHOULD BE SET AS FOLLOWS)
      RETURN
      END
```

```
C       OPTION TO SET POT VALUES
        SUBROUTINE PARSET(IX,PS)
        COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
       1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
       2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
       3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
       4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
        DIMENSION PT(16)
        DATA PT(1),PT(2),PT(3),PT(4),PT(5),PT(6),PT(7),PT(8),PT(9),PT(10),
       1PT(11),PT(12),PT(13),PT(14),PT(15),PT(16)
       2    /4HP010,4HP011,4HP012,4HP013,4HP014,4HP015,4HP016,4HP017,
       34HP018,4HP019,4HP020,4HP021,4HP022,4HP023,4HP024,4HP025/
        GO TO(1,2,2,3,4,2,2,2,2,2,2,2,2,2,5,1),IX
      1 CONTINUE
        GO TO 10
      2 PVAL=PS
        IXP=IX
        CALL POTST(IXP,PVAL,PT)
        GO TO 10
      3 IXP=4
C       FIELD CAPACITY =DIG(3)
        PVAL=PS/SKAL
        DIG(3)=PS
        CALL POTST(IXP,PVAL,PT)
        GO TO 10
      4 IXP=5
        PVAL=PS/SKAL
        CALL POTST(IXP,PVAL,PT)
        GO TO 10
      5 IXP=15
C       CRITICAL MOISTURE CONTENT =DIG(2)
        DIG(2)=PS
        PVAL=PS/SKAL
        CALL POTST(IXP,PVAL,PT)
     10 RETURN
        END


        SUBROUTINE POTST (IXP,PVAL,PT)
        COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
       1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
       2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
       3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
       4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
        DIMENSION PT(16)
        PADR=PT(IXP)
        GO TO(4,4,4,4,4,1,2,3,4,4,4,4,4,4,4),IXP
      1 PVAL=PVAL/(1.6*TI**2)
        GO TO 4
      2 PVAL=PVAL/(TI*4.)
        GO TO 4
      3 PVAL=PVAL/(TI*6.)
      4 CALL OWPR(PADR,PVAL,IERR)
        RETURN
        END
```

```
C       SUBROUTINE FOR ARITHMATIC PLOTTING
        SUBROUTINE GRAPH
        COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
       1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
       2NL(25),NYR,XXX,OBI(25),OBS(2,25),PCP(9),PDL(12),PH(25),PL(25),
       3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
       4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
        DATA XSCALE,YSCALE,XREF,YREF,XVAL,YVAL,XP,YP,XN,YN/1.,1.,0.,0.,
       10.,0.,24.,7.,0.,0./
        CALL PLTSET(XSCALE,YSCALE,XREF,YREF,XVAL,YVAL,XP,YP,XN,YN)
C       DRAW XAXIS YAXIS
        TYPE 100
    100 FORMAT(13HREADY PLOTTER/)
C       PAUSE
        OCT 25000
        CALL SBYSET
        CALL PENDN
        CALL INPLOT(24.,0.)
        CALL PENUP
        CALL INPLOT(0.,0.)
        CALL PENDN
        CALL INPLOT(0.,7.)
        CALL PENUP
        CALL PLOT(0.,0.)
C       PLOTTING OBSERVED FLOW
        IX=0
        DO 10 K=1,2
        DO 10 IM=1,12
        IF(K.GT.1) IX=12
        X=IX+IM
        Y=OBS(K,IM)
        CALL PLOT(X,Y)
        CALL PENDN
     10 CONTINUE
        CALL PENUP
        CALL PLOT(0.,0.)
C       PLOTTING SIMULATED FLOW
        TYPE 101
    101 FORMAT(10HCHANGE PEN/)
C       PAUSE
        OCT 25000
        IX=0
        DO 15 K=1,2
        DO 15 IM=1,12
        IF(K.GT.1) IX=12
        X=IX+IM
        Y=SIM(K,IM)
        CALL PLOT(X,Y)
        CALL PENDN
     15 CONTINUE
        CALL PENUP
        RETURN
        END
```

```
C     SUBROUTINE QUAL
      SUBROUTINE QUAL
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(2[illegible]),[illegible]3(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      COMMON/BLK3/PCA(24,5),PCL(24,5),PHCO3(24,5),PMG(24,5),PNA(24,5),
     1PNO3(24,5),PSO4(24,5),OBJ,CCA(70),CMG(70),CNA(70),CCL(70),
     2CHCO3(70),CSO4(70),CCNO3(70)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      READ(6,120) NS,NMO,ITX,III
      READ(6,125) (CO(I),I=1,NS)
  120 FORMAT(I2,I3,2I2)
  125 FORMAT(5F6.2)
      CALL CONINP(III)
      CALL UPTAKE
      DO 3000 NN=1,NS
      CALL SOIL
      XM=MM
      DDP=0.
      L=0
C     LL=COUNTER TO CHECK FRACTIONAL VOLUMES OF DP
      LL=0
C     IS LIME PRESENT
      DO 448 J=1,MM
      ZE(J)=2.E-8
      IF(XLIME(J).EQ.0.) GO TO 448
      U=SQRT(2.*(TCA(J)+TMG(J)+TSO4(J))+.5*(TNA(J)+TCL(J)+THCO3(J)+
     1TNO3(J)))
      ZE(J)=TCA(J)*THCO3(J)**2*EXP(-2.341*U/(1.+U))
  448 CONTINUE
C     L IS THE MONTH
  200 L=L+1
      MN=L
      IF(L-NMO) 2005,2005,933
C     CONVERT MOL/L TO ME/L
 2005 UREA=TUREA(1)
      AN=TNO3(1)*CF1
      ANH3=TNH3(1)*CF1
      A=TCA(1)
      G=TSO4(1)
      IF(ITX) 2,2,3
    2 WRITE(6,5) AN,ANH3,A,G
    5 FORMAT(4E10.4)
    3 CONTINUE
      CALL TRNSFM(MN)
      TNO3(1)=(AN-PLNO3(MN))/CF1
      TNH3(1)=(ANH3-PLNH4(MN))/CF1
      IF(TNO3(1).LE.0.) TNO3(1)=0.
      IF(TNH3(1).LE.0.) TNH3(1)=0.
      TUREA(1)=AAMT(2,1)
      TSO4(1)=G
      TCA(1)=A
      TNH4(1)=BNH4
      IF(ITX) 4,4,6
    4 WRITE(6,5) TNO3(1),TNH3(1),TSO4(1),TNH4(1)
    6 CONTINUE
      DDP=DDP+DP(L)
C     NUMBER OF PORE VOLUMES OF DP
      XN=DDP/PV
      XK=1./XM
      WRITE(6,20) L,XN,XK
   20 FORMAT(/7H MONTH=,I3,3X,3HXN=,F7.3,3X,3HXK=,F7.3/)
      IF(XK.LE.XN) GO TO 204
 2006 IF(DAL(L).LE.0.) GO TO 2031
C     NUMBER OF PORE VOLUMES OF DAL APPLIED TO TOP LAYER=RQ
      RQ=DAL(L)*XM/PV
C     RESULTANT    CONC OF IONS IN TOP LAYER
      TCA(1)=TCA(1)+CA(L)*RQ
      TMG(1)=TMG(1)+AMG(L)*RQ
      TNA(1)=TNA(1)+ANA(L)*RQ
      TCL(1)=TCL(1)+CL(L)*RQ
      THCO3(1)=THCO3(1)+HCO3(L)*RQ
      TSO4(1)=TSO4(1)+SO4(L)*RQ
      TNO3(1)=TNO3(1)+CNO3(L)*RQ
      TNH3(1)=TNH3(1)+TTNH3(L)*RQ
      GO TO 200
 2031 IF(SMCH(L).GT.0.) GO TO 2032
      SMCH(L)=ABS(SMCH(L))
      CCF=SMCH(L)*XM/PV
      IF(CCF.LT.1.) CCF=1.0
      GO TO 2033
C     NUMBER OF PORE VOLUMES OF DILF TO TOP LAYER CCF
 2032 CCF=PV/(XM*SMCH(L))
      IF(CCF.GT.1.) CCF=1.
C     CHANGE IN CONC OF TOP LAYER DUE TO CHANGE IN MOISTURE
 2033 TCA(1)=TCA(1)*CCF
      TMG(1)=TMG(1)*CCF
      TNA(1)=TNA(1)*CCF
      TCL(1)=TCL(1)*CCF
      THCO3(1)=THCO3(1)*CCF
      TSO4(1)=TSO4(1)*CCF
      TNH3(1)=TNH3(1)*CCF
      TNO3(1)=TNO3(1)*CCF
      GO TO 200
  204 DDP=0.
  203 FK=0.
  201 J=0
C     CHECK IF NO APPRECIABLE DAL
      IF(DAL(L).LE..01) GC TO 2111
C     ADJUST CONCENTRATIONS IN APPLIED WATER PRIOR TO PERCOLATION
      FF=DP(L)/DAL(L)
      A=CA(L)/FF
      F=AMG(L)/FF
      S=ANA(L)/FF
      G=SO4(L)/FF
      H=CL(L)/FF
      W=HCO3(L)/FF
      AN=CNO3(L)/FF
      ANH3=TTNH3(L)/FF
      GO TO 2027
 2111 A=0.
      F=0.
      S=0.
      G=0.
```

```
      H=0.
      W=0.
      PO=0.
      AN=0.
      ANH3=0.
 2027 CASO=0.
      AGSO=0.
  202 J=J+1
      KK=2
      IF(XLIME(J).LE..00001) KK=1
      TES=.000001
C     RATIO OF GRAMS OF SOIL TO LITER OF SOIL SOLUTION
      B=TB(J)
      A=(A+TCA(J))/2.
      F=(F+TMG(J))/2.
      S=(S+TNA(J))/2.
      G=(G+TSO4(J))/2.
      H=(H+TCL(J))/2.
      W=(W+THCO3(J))/2.
      CASO=(CASO+TCASO(J))/2.
      AGSO=(AGSO+TAGSO(J))/2.
      ET=TE(J)
      CT=TC(J)
      SAT=TSO(J)
      AN=(AN+TNO3(J))/2.
      ANH3=(ANH3+TNH3(J))/2.
C     CONVERT XXT FROM MEQ/100GM TO MOL/GM
      XXT=TXX(J)/2.E5
  605 CALL XCHNGE(J,A,F,S,H,G,W,CASO,AGSO,XXT,B,SAT,ET,
     1TES,KK,CT,AN,ANH3,BNH4,DNH4)
C     EQUILIBRIUM CONCENTRATIONS OF IONS IN MOLES/L
      TCA(J)=A
      TMG(J)=F
      TNA(J)=S
      TSO4(J)=G
      TCL(J)=H
      THCO3(J)=W
      TCASO(J)=CASO
      TAGSO(J)=AGSO
      TXX(J)=XXT
      TE(J)=ET
      TC(J)=CT
      TSO(J)=SAT
      TNO3(J)=AN
      TNH3(J)=ANH3
C     CHECK TO SEE THAT ALL LAYERS ARE ROUTED
   77 IF(J-MM) 202,10,10
   10 LL=LL+1
C     LL COUNTS NUMBER OF FRACTIONAL PORE VOLUMES OF EFFLUENT
      IF(LL.GT.70) TYPE 5099,LL
 5099 FORMAT(24HDIMENSION OVERFLOW LL=  ,I3)
C     STORE EQULIBRIUM CONCENTRATIONS OF EACH MONTH IN MEQ/L
      CCA(LL)=TCA(J)*CF2
      CMG(LL)=TMG(J)*CF2
      CNA(LL)=TNA(J)*CF1
      CCL(LL)=TCL(J)*CF1
      CHCO3(LL)=THCO3(J)*CF1
      CSO4(LL)=TSO4(J)*CF2
      CCNO3(LL)=TNO3(J)*CF1
C     FK COUNTS THE NUMBER OF FRACTIONAL PORE VOLUMES OF DP MONTH JJ
      FK=FK+1./XM
C     CHECK TO SEE THAT ALL DP IS ROUTED
      IF(FK-XN) 201,334,334
```

```
C     CHECK TO SEE THAT ALL MONTHS ARE ROUTED
  334 IF(L-NMO) 200,933,933
  933 WRITE(6,5003)
 5003 FORMAT(//51H QUALITY OF PERCOLATED EFFLUENT IN ME/L TDS IN MG/L)
      WRITE(6,5111)
      CALL AVQLTY
 3000 CONTINUE
C     COMPUTE WEIGHTED CONC OF EFFLUENT IN EACH SOIL
      CALL SALT
 5111 FORMAT(/6H MONTH,4H  CA,6X,2HMG,6X,2HNA,5X,3HSO4,6X,2HCL,4X,
     14HHCO3,6X,3HNO3,4X,3HTDS,5X,4HSOIL/)
      RETURN
      END
```

```
C     SUBROUTINE TO PREDICT UPTAKE OF NO3 AND NH4
      SUBROUTINE UPTAKE
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C     CONVERT LBS/ACRE TO MEQ/L
      UK1=0.95
      UK2=0.05
      DO 5 J=1,NMO
      UPTK(J)=UPTK(J)*CCC*P/(BD*DELX*14.*(1.-P))
C     ADJUST UPTAKE TO AVAILABLE MOISTURE
      U1(J)=UPTK(J)*SM(J)/FMCS
C     PROPORTION UPTK BETWEEN NO3 AND NH4
      PLNO3(J)=U1(J)*UK1
      PLNH4(J)=U1(J)*UK2
    5 CONTINUE
      IF(ITX) 6,6,30
    6 WRITE(6,8)
      DO 20 J=1,NMO
      WRITE(6,10) J,PLNO3(J),PLNH4(J)
   20 CONTINUE
    8 FORMAT(6H MONTH,5X,5HPLNO3,5X,5HPLNH4/)
   10 FORMAT(I8,2E10.4)
   30 CONTINUE
      RETURN
      END
```

```
C     SUBROUTINE FOR INPUT PARAMETERS
      SUBROUTINE CONINP(III)
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      AREA=202700.
      CF1=1000.
      CF2=2000.
C     READ INFLOW SURFACE WATERS CONCENTRATION IN MOL/L
      READ(6,100) (CA(I),AMG(I),ANA(I),SO4(I),CL(I),HCO3(I),AK(I),
     1CNO3(I),TTNH3(I),I=1,NMO)
C     READ PARAMETERS FROM HYDSM
      IF(III) 6,6,5
    5 READ(6,105) (SRF(I),SUBSRF(I),GWBF(I),SNPC(I),DAL(I),STRC1(I),
     1DP(I),SUMOUT(I),SMCH(I),SM(I),I=1,NMO)
      WRITE(6,105)(SRF(I),SUBSRF(I),GWBF(I),SNPC(I),DAL(I),STRC1(I),
     1DP(I),SUMOUT(I),SMCH(I),SM(I),I=1,NMO)
C     READ SURFACE WATER OUTFLOW CONC
    6 WRITE(6,50)
      DO 115 J=1,NMO
      READ(6,110) (X1(I),I=1,7)
  195 WRITE(6,55)(J,(X1(I),I=1,7))
      X3(J)=0.
      DO 115 K=1,7
  115 X3(J)=X3(J)+X1(K)
      IF(ITX) 190,190,200
  190 WRITE(6,30)
      WRITE(6,35)
      WRITE(6,40)(I,CA(I),AMG(I),ANA(I),SO4(I),CL(I),HCO3(I),AK(I),
     1CNO3(I),TTNH3(I),I=1,NMO)
   30 FORMAT(42H INFLOW SURFACE WATER CONCENTRATION-MOLS/L/)
   35 FORMAT(51H MON      CA         MG         NA         SO4        CL,
     120H       HCO3       K/,
     220H        NO3       NH3/)
   40 FORMAT(I3,7E10.3/3X,2E10.3)
   50 FORMAT(33H OBSERVED SURFACE OUTFLOW IN TONS/)
   55 FORMAT(I3,7F10.1/)
  100 FORMAT(7E10.3/2E10.3)
  105 FORMAT(10F6.2)
  110 FORMAT(7F7.1)
  200 CALL ANDAT
      RETURN
      END
```

```
      SUBROUTINE ANDAT
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      CCC=11.221367
      FMCS=8.0
C     READ COEFFICIENTS FOR NITROGEN TRANSFORMATION RATE EQUATIONS
      READ(6,30) (C(I),I=1,4)
      READ(6,30) (B1(I),I=1,4)
      READ(6,30)(B2(I),I=1,4)
      READ(6,30) (B3(I),I=1,4)
      DO 200 I=1,4
      CC(I)=C(I)
      BB1(I)=B1(I)
      BB2(I)=B2(I)
  200 BB3(I)=B3(I)
      READ(6,10) RN(1),RC(1),P,D1,CNR,DA,D,DNH4,BD,DELX,DELT
C     READ FERTILIZER APPLICATIONS ON SOIL SURFACE IN LBS/ACRE
      READ(6,160) (AUREA(I),I=1,NMO)
      READ(6,160) (AANH3(I),I=1,NMO)
      READ(6,160) (AANO3(I),I=1,NMO)
      READ(6,160) (AACA(I),I=1,NMO)
      READ(6,160) (AACO3(I),I=1,NMO)
      READ(6,160) (AASO4(I),I=1,NMO)
      READ(6,160) (AOR(I),I=1,NMO)
      READ(6,160) (UPTK(I),I=1,NMO)
      READ(6,160) (T(I),I=1,NMO)
      READ(6,160)(UBIOM(I),I=1,NMO)
      DO 210 I=1,NMO
      AOR(I)=AOR(I)*CCC/(BD*DELX)
  210 TEN(I)=-(1.013)*SM(I)/(3.*FMCS)
C     CONVERT TO UG/GM FROM PERCENT RESIDUE N AND C
      RN(1)=RN(1)*1.0E4
      RC(1)=RC(1)*1.0E4
      ORN=RN(1)
      IF(ITX) 250,250,260
  250 WRITE(6,25)FMCS,SM(1),RN(1),RC(1),CNR,DA,D,BD,DELX,DNH4,DELT
      WRITE(6,35)
      DO 170 I=1,NMO
  170 WRITE(6,180)I,AANH3(I),AANO3(I),AUREA(I),AACA(I),AACO3(I),
     1AASO4(I),AOR(I),UPTK(I),T(I),UBIOM(I)
   10 FORMAT(13F6.2)
   25 FORMAT(2F6.2,F7.3,2F6.2,2F6.2,3F6.2,F7.3)
   30 FORMAT(4E10.3)
   35 FORMAT(/50H MO ANH4   AANO3  AUREA  AACA   AACO3  AASO4   AOR,
     121H    UPTK     T   UBOIM)
  160 FORMAT(12F6.2)
  180 FORMAT(I3,10F7.3)
  260 CONTINUE
      RETURN
      END
```

```
C     SUBROUTINE FOR EQUIL-CONC OF IONS IN INITIAL SOIL SOLUTIIN
      SUBROUTINE EQEXCH(I,U)
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(22),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      CA=TCA(I)
      AMG=TMG(I)
      SOS=TNA(I)
      CL=TCL(I)
      SO4=TSO4(I)
      HCO3=THCO3(I)
      ANO3=TNO3(I)
      E5=TE(I)
      C5=TC(I)
      SA5=TSO(I)
      CASO=TCASO(I)
      AGSO=TAGSO(I)
      BE=EC(I)
      CASO=0.
C     IONIC STRENGTH-  U=U**.5
      U=SQRT(2.*(CA+AMG+SO4)+.5*(SOS+CL+HCO3+ANO3))
      AGSO=0.
   42 ACT2=EXP(-9.366*U/(1.+U))
      IF(SO4) 713,713,712
  712 AA=ACT2*ACT2
      BB=ACT2*(10.8E-3+(ACT2*(AMG+CA-SO4)))
      CC=28.91E-6+(ACT2*(AMG*4.9E-3+(CA*5.9E-3)-(SO4*10.8E-3)))
      DD=-SO4*28.91E-6
  800 Z=SO4/2.
  850 Z1=Z
  863 ZZ=-(((AA*Z+BB)*Z+CC)*Z+DD)
      ZZZ=((3.*AA*Z+2.*BB)*Z+CC)
      ZZ=ZZ/ZZZ
      ZZZ=ZZ/Z
      Z=Z+ZZ
      IF(ABS(ZZZ)-.001) 840,840,863
  840 SO4T=SO4
      SO4=Z
      IF(SO4) 710,710,711
  710 SO4=SO4T
      Z=Z1
      GO TO 863
  711 CASX=SO4*CA*ACT2/(4.9E-3+ACT2*SO4)
      CX=CA-CASX
      AGSX=SO4*AMG*ACT2/(5.9E-3+ACT2*SO4)
      AMX=AMG-AGSX
      UU=SQRT(2.*(CX+AMX+SO4)+.5*(SOS+HCO3+CL+ANO3))
      IF(ABS(UU/U-1.)-1.0E-4) 40,40,41
   41 U=UU
      SO4=SO4T
      GO TO 42
   40 CASO=CASX
      AGSO=AGSX
      CA=CX
      AMG=AMX
  713 ACT1=SQRT(ACT2)
      ACTM=SQRT(ACT1)
      ACTN=SQRT(ACTM)
      CA=CA*2.
      AMG=AMG*2.
C     CA MG ARE IN EQ/L
C     EXCHANGEABLE CALCIUM
      E5=BE/((ACTM*SOS/(DA*SQRT(ACT1*CA)))+1.+(D*ACT1*AMG/(ACT1*CA)))
C     EXCHANGEABLE NA
      SA5=ACTM*SOS*E5/(SQRT(ACT1*CA)*DA)
C     EXCHANGEABLE MAGNESIUM
      C5=BE-E5-SA5
C     CONVERT ET ANDCT TO MOL/GM  A AND F TO MOL/L
      E5=E5/2.
      C5=C5/2.
      CA=CA/2.
      AMG=AMG/2.
      TCA(I)=CA
      TMG(I)=AMG
      TNA(I)=SOS
      TCL(I)=CL
      TSO4(I)=SO4
      THCO3(I)=HCO3
      TE(I)=E5
      TC(I)=C5
      TSO(I)=SA5
      TCASO(I)=CASO
      TAGSO(I)=AGSO
      TNO3(I)=ANO3
      EC(I)=BE
      RETURN
      END
```

```
C     SUBROUTINE FOR COMPUTING PRECIPITATION AND TEMP DATA
C     THIS SUBROUTINE IS REQUIRED IF DATA OF PRECIP AND TEMP IS
C     DIFFERENT FROM THAT OF FIRST YEAR
      SUBROUTINE PRETEM(L)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),OP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      COMMON/BLK5/AB(9),AGINIC,ARF1,B(9),CAC(9),DDA(6),DCA(9),DD(12),
     1DF(25),DIG(12),DUM(2,12,8),EFF(12),FK(12),I,II,I1(9),J,JJ,LYRO,
     2NL(25),NYR,XXX,OBI(25),OPS(2,25),PCP(9),PDL(12),PH(25),PL(25),
     3PM(25),PR(25),PVV(25),SCAC,SIM(2,25),SKAL,SNO,SWKC(12),TI,
     4XIN(6,25),XMN(25),XPM(25),VV(13),WKC(9,12),EVT(24)
      IF(II-1) 50,50,60
   50 DO 51 JJ=1,12
      READ(6,100) T1,T2,T3
      DD(JJ)=(T1+T2+T3)/3.
      DUM(II,JJ,J)= DUM(II,JJ,J)+DD(JJ)
      IF(J.EQ.8) DUM(II,JJ,J)=(DUM(II,JJ,J))/100.
   51 CONTINUE
      GO TO 70
   60 READ(6,100)(DD(JJ),JJ=1,12)
      DO 61 JJ=1,12
      DUM(II,JJ,J)= DUM(II,JJ,J)+DD(JJ)
      IF(J.EQ.8) DUM(II,JJ,J)=(DUM(II,JJ,J))/100.
   61 CONTINUE
   70 IF(J-8) 71,72,72
   71 WRITE(6,230) J,L,(DUM(II,JJ,J),JJ=1,12)
      GO TO 250
   72 WRITE(6,231) J,L,(DUM(II,JJ,J),JJ=1,12)
  100 FORMAT(12F6.1)
  230 FORMAT(1XI2,I5,9F8.2/8X,3F8.4)
  231 FORMAT(1XI2,I5,9F8.2/8X,3F8.2)
  250 RETURN
      END
```

```
C     SUBROUTINE FOR INITIAL EGUILIBRIUM CONCENTRATION OF SOIL SOLN
      SUBROUTINE SOIL
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,DAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C     READ NUMBER OF SOIL LAYERS AND PORE VOLUMES
      READ(6,140)MM,PV
C     READ SOIL CHARACTERISTICS IN ME/L
      READ(6,145) (TCA(I),TMG(I),TNA(I),TK(I),THCO3(I),TCL(I),TSO4(I),
     1EC(I),TE(I),TC(I),TSO(I),TXX(I),XLIME(I),TB(I),TCASO(I),
     2TNO3(I),TNH3(I),TUREA(I),TAGSO(I),I=1,MM)
      READ(6,160) (TNH4(I),I=1,MM)
      WRITE(6,130)
      WRITE(6,155)(TCA(I),TMG(I),TNA(I),TK(I),TCL(I),TSO4(I),
     1THCO3(I),EC(I),TE(I),TC(I),TSO(I),TCASO(I),TAGSO(I),
     2TNO3(I),TNH3(I),TUREA(I),I=1,MM)
  130 FORMAT(40H CONCENTRATIONS OF INITIAL SOIL SOLUTION/)
  140 FORMAT(I2,F6.2)
  145 FORMAT(11F6.2/8F6.2)
  160 FORMAT(7E10.3/7E10.3/7E10.3)
C     CONVERT ME/L TO MOL/L
      DO 150 I=1,MM
      TCA(I)=TCA(I)/CF2
      TMG(I)=TMG(I)/CF2
      TNA(I)=TNA(I)/CF1
      TK(I)=TK(I)/CF1
      TCL(I)=TCL(I)/CF1
      TSO4(I)=TSO4(I)/CF2
      THCO3(I)=THCO3(I)/CF1
      TNH3(I)=TNH3(I)/CF1
      TNO3(I)=TNO3(I)/CF1
C     CONVERT CEC FROM MEQ/100GMS TO EQ/GM
      EC(I)=EC(I)/1.0E5
      CALL EQEXCH(I,U)
  150 CONTINUE
      IF(ITX) 1,1,161
    1 WRITE(6,151)
  151 FORMAT(/52H EQUILIBRIUM CONCENTRATIONS OF INITIAL SOIL SOLUTION/)
      WRITE(6,155)(TCA(I),TMG(I),TNA(I),TK(I),TCL(I),TSO4(I),
     1THCO3(I),EC(I),TE(I),TC(I),TSO(I),TCASO(I),TAGSO(I),
     2TNO3(I),TNH3(I),TUREA(I),I=1,MM)
  155 FORMAT(/2X,7E10.4/2X,7E10.4/2X,2E10.4/)
  161 CONTINUE
      RETURN
      END
```

```
C     SUBROUTINE TO PREDICT NITHOGEN TRANSFORMATIONS
      SUBROUTINE TRNSFM(N)
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(22),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,DAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C     COMPONENT UNITS ARE IN UG/SEGMENT
C     SOIL TEMPERATURES IN DEGREE C . MOISTURE IN BARS
C     RATE UNITS ARE IN UG/GRAM OF SOIL/DAY
C     +VE RATE IS GAIN. -VE RATE IS LOSS WITH RESPECT TO THE
C     PARTICULAR CONSTITUENT
C     SET INITIAL VALUES
      MN=N
      M=1
      K=1
      J=1
      PVV=P*D1
C     CONVERT MEQ/L TO UG/SEGMENT OF NO3 AND AMMONIA IN SOLUTION
      AN=AN*(1.-P)*14.*BD*DELX/P
      ANH3=ANH3*(1.-P)*DELX*BD*14.0/P
C     CONVERT MOLES/G TO UG/SEGMENT OF EXCHANGEABLE AMMONIUM
      BNH4=TNH4(1)
      ENH4=BNH4*DELX*BD*14.0E6
      CONVRT=BD*DELX
C     CONVERT TO UG/SEGMENT AT PORE VOLUME SATURATION
      CCC=11.221367
      SAVE1=AANH3(N)*CCC*0.7777
      SAVE2=AANO3(N)*CCC*0.2258
      SAVE3=AUREA(N)*CCC
      SAVE4=AACA(N)*CCC
      SAVE9=AACO3(N)*CCC
      SAVE10=AASO4(N)*CCC
C     ADD THE FERTILIZER TO PROPER ARRAYS
      ANH3=ANH3+SAVE1
      AN=AN+SAVE2
      UREA=UREA+SAVE3
C     CONVERT MOL/L TO UG/SEGMENT OF SOIL SOLUTION
      A=A*PVV*40080.+SAVE4
      G=G*PVV*96100.+SAVE10
C     CONVERT TO UG/GM OF SOIL FROM UG/SEGMENT VOLUME
      ANH3=ANH3/CONVRT
      AN=AN/CONVRT
      UREA=UREA/CONVRT
      A=A/CONVRT
      G=G/CONVRT
      ENH4=ENH4/CONVRT
      AAMT(1,1)=UREA
      AAMT(1,2)=ORN
      AAMT(1,3)=ANH3+ENH4
      AAMT(1,4)=AN
      SAMT(1,1)=0.
      SAMT(1,2)=AOR(N)
      SAMT(1,3)=0.
      SAMT(1,4)=0.
      AAMTRN(1)=RN(1)
```

```
      V(1)=ABS(TEN(N))
      AAMTRC(1)=RC(1)
      CN1(1)=CNR
C     ENTER LOOP TO DO COMPUTATIONS FOR EACH TIME INTERVAL
  612 DO 611 I=1,K
C     UREA HYDROLYSIS
      L=1
      AMT(1,1)=AAMT(M,L)+SAMT(M,L)
C     CHECK FOR ZERO AMOUNT OF UREA-N
      IF(AMT(I,1).EQ.0.0) GO TO 310
      GO TO 801
C     SET RATE EQUAL TO ZERO FOR ZERO AMOUNT OF UREA-N
  310 R(I,L)=0.
      GO TO 311
  801 CALL RATE1 (I,L,N)
  311 AMT(I+1,L)=AMT(I,L)+R(I,L)
      IF(AMT(I+1,L))615,616,616
  615 AMT(I+1,L)=0.
C     ENTER ORGANIC-N ROUTINE
  616 L=2
C     COMPUTE AMOUNT OF ORGANIC-N ADDED
      IF(CN1(M).EQ.0.) OAMT(M,L)=0.
      IF(CN1(M).GT.0.) OAMT(M,L)=0.4/CN1(M)*SAMT(M,2)
C     COMPUTE THE AMOUNTS OF ORG-N,NH4-N,NO3-N PRESENT AT START
      AMT(1,L)=OAMT(M,L)+AAMT(M,2)
      AMT(1,3)=SAMT(M,3)+AAMT(M,3)
      AMT(1,4)=SAMT(M,4)+AAMT(M,4)
      IF(AMT(I,3).EQ.0.0) AMT(I,3)=0.0001
C     COMPUTE INITIAL AMOUNTS OF RESIDUAL-N AND RESIDUE-C
      IF(CN1(M).EQ.0.0) AMTRN(1)=AAMTRN(M)
      IF(CN1(M).GT.0.0) AMTRN(1)=0.4/CN1(M)*SAMT(M,2)+AAMTRN(M)
      IF(CN1(M).EQ.0.0) AMTRC(1)=AAMTRC(M)
      IF(CN1(M).GT.0.0) AMTRC(1)=0.4*SAMT(M,2)+AAMTRC(M)
      IF(AMTRC(1).LE.0.0.OR.AMTRN(1).LE.0.0) GO TO 202
      GO TO 203
  202 CN(1)=10.0
      GO TO 204
  203 CN(1)=AMTRC(1)/AMTRN(1)
C     MAKE CONSTANT ADJUSTMENT ACCORDING TO C/N RATIO
  204 IF(CN(1).LT.23.0) B2(3)=4.5
      IF(CN(1).LT.23.0) B3(2)=1.6
      IF(CN(1).GE.23.0) B3(2)=.7832
      IF(CN(1).GE.23.0) B1(3)=.0008
      IF(CN(1).GE.23.0) B2(3)=.0002384
      IF(CN(1).GE.23.0) B3(3)=-2.1
  751 CALL RATE2 (I,L,N)
      IF(R(I,L)) 802,803,804
  802 IF(AMT(I,L).LT.ABS(R(I,L))) R(I,L)=-AMT(I,2)
      GO TO 803
  804 IF(AMT(I,3).LT.R(I,L)) R(I,L)=AMT(I,3)
C     ADJUST RATE FOR LENGTH OF TIME INTERVAL
  803 R(I,L)=R(I,L)/DELT
      IF(AMT(I,2).EQ.0.0) AMT(I,2)=0.0001
C     CHECK FOR ZERO AMOUNT OF NO3-N
      IF(AMT(I,4).EQ.0.0) GO TO 307
      GO TO 308
  307 R(I,5)=0.0
      GO TO 309
  308 CALL RATE3 (I,L,N)
C     ENTER BRANCH ACCORDING TO C/N RATIO
  309 IF(CN(I).LE.80.0.AND.CN(I).GT.23.0) GO TO 200
      GO TO 201
C     COMPUTE AMOUNT OF RESIDUE-C AT T+1
  200 AMTRC(I+1)=AMTRC(I)-(30.0*(R(I,L)+R(I,5)))
C     COMPUTE RESIDUE-N AT T+1
      AMTRN(I+1)=AMTRN(I)
      IF(AMTRC(I+1).LE.0.0.OR.AMTRN(I+1).LE.0.0) GO TO 1030
      GO TO 1031
C     COMPUTE AMOUNT OF RESIDUE-N AND RESIDUE-C AT T+1
  201 AMTRC(I+1)=AMTRC(I)-(30.0*(ABS(R(I,L)-R(I,5))))
      AMTRN(I+1)=AMTRN(I)-ABS(R(I,L))
      IF(AMTRC(I+1).LE.0.0.OR.AMTRN(I+1).LE.0.0) GO TO 1030
      GO TO 1031
 1030 CN(I+1)=10.0
      GO TO 1022
C     COMPUTE C/N RATIO AT T+1
 1031 CN(I+1)=AMTRC(I+1)/AMTRN(I+1)
 1022 IF(AMTRC(I+1).LE.0.0) AMTRC(I+1)=0.0
      IF(AMTRN(I+1).LE.0.0) AMTRN(I+1)=0.0
      IF(I.EQ.K) AAMTRN(M+1)=AMTRN(I+1)
      IF(I.EQ.K) AAMTRC(M+1)=AMTRC(I+1)
      AMT(I+1,L)=AMT(I,L)+R(I,L)+R(I,5)
      IF(AMT(I+1,L)) 620,621,621
  620 AMT(I+1,L)=0.0
C     ENTER AMMONIA-N ROUTINE
  621 L=3
      IF(AMT(I,4).EQ.0.0) AMT(I,4)=0.0001
C     CHECK FOR ZERO AMOUNT OF NH4-N
      IF(AMT(I,3).EQ.0.0) GO TO 305
      GO TO 753
  305 R(I,L)=0.0
      GO TO 306
  753 CALL RATE4 (I,L,N)
C     COMPUTE AMOUNT OF NH3-N PRESENT AT T+1
  306 AMT(I+1,L)=AMT(I,L)-R(I,1)-R(I,2)-R(I,3)
      IF(AMT(I+1,L)) 622,623,623
  622 AMT(I+1,L)=0.0
C     ENTER NO3-N ROUTINE
  623 L=4
C     COMPUTE AMOUNT OF NO3-N PRESENT AT T+1
      IF(R(I,5).GT.R(I,3)) GO TO 900
      GO TO 901
  900 IF(CN(I).LE.10.0.AND.AMT(I,4).LE.6.0)AMT(I+1,2)=AMT(I+1,2)-(R(I,5)
     1-R(I,3))
      IF(CN(I).LE.10.0.AND.AMT(I,4).LE.6.0) R(I,5)=R(I,3)
  901 CONTINUE
      AMT(I+1,L)=AMT(I,L)+R(I,3)-R(I,5)
      IF(AMT(I+1,L)) 624,625,625
  624 AMT(I+1,L)=0.0
  625 CONTINUE
  611 CONTINUE
C     COMPUTE AMOUNTS FOR START OF NEXT TIME STEP
      DO 632 L=1,4
  632 AAMT(M+1,L)=AMT(K+1,L)
      CNR=CN(2)
      RN(1)=AAMTRN(2)
      RC(1)=AAMTRC(2)
      ORN=RN(1)
C     CONVERT UNITS TO UG/SEGMENT FROM UG/G
      DO 60 J=1,4
      AAMT(1,J)=AAMT(1,J)*CONVRT
   60 AAMT(2,J)=AAMT(2,J)*CONVRT
      RATIO=AAMT(2,3)/AAMT(1,3)
      FIRST=AAMT(1,3)-ENH4*CONVRT
      FINAL=FIRST*RATIO
      FINAL1=BNH4*RATIO
```

```
      BNH4=FINAL1
C     CONVERT AN AND ANH3 TO MEQ/L
      AN=AAMT(2,4)*P/((1.-P)*14.*BD*DELX)
      ANH3=FINAL*P/((1.-P)*14.*BD*DELX)
C     CONVERT A AND G TO MOL/L
      A=(A*CONVRT)/(PVV*40080.)
      G=(G*CONVRT)/(PVV*96100.)
      UREA=AAMT(2,1)
      IF(ITX) 61,61,62
   61 DO 50 I=1,2
      WRITE(6,10) (AAMT(I,J),J=1,4)
      WRITE(6,10) (R(I,J),J=1,5)
      WRITE(6,10) (AMT(I,J),J=1,4)
      WRITE(6,10) (SAMT(I,J),J=1,4)
      WRITE(6,10) AAMTRN(I)
      WRITE(6,10) CN(I)
   50 WRITE(6,10) AAMTRC(I)
      WRITE(6,15) CNR,RN(1),RC(1),BNH4,AN,ANH3,UREA
   10 FORMAT(6F12.2)
   15 FORMAT(7E10.3)
   62 CONTINUE
      L=MN
      RETURN
      END
```

```
      SUBROUTINE RATE3(I,L,M)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C     COMPUTE RATE OF NO3-N IMMOBILIZATION
  308 R(I,5)=(B1(4)*EXP(T(M)))+(B2(4)*T(M)/AMT(I,2)**2)+(B3(4)*
     1(T(M)*(AMT(I,2)-AMT(I,4)))/AMT(I,2))
      IF(CN(I).LE.10.0) GO TO 1
      GO TO 5
    1 R(I,5)=R(I,5)*0.1
      R(I,2)=R(I,2)*0.005
    5 CONTINUE
C     CORRECT RATE FOR LOW TEMP
      IF(T(M).LE.10.0) R(I,5)=R(I,5)*ALOG10(T(M))/4.0
C     CORRECT RATE FOR LOW MOISTURES
      IF(V(I).GE.10.0) R(I,5)=R(I,5)/ALOG10(V(I))*0.3
  809 IF(AMT(I,4).LT.R(I,5)) R(I,5)=AMT(I,4)
      IF(R(I,5).LE.0.0) R(I,5)=ABS(R(I,5))
C     ADJUST RATE FOR LENGTH OF TIME INTERVAL
  808 R(I,5)=R(I,5)/DELT
      RETURN
      END
```

```
      SUBROUTINE RATE4 (I,L,M)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C     COMPUTE RATE OF NITRIFICATION
  753 R(I,L)=C(L)+(B1(L)*T(M)*AMT(I,3))+(B2(L)*ALOG10(AMT(I,3)))+(B3(L)*
     1ALOG10(AMT(I,4)))
C     CORRECT RATE FOR LOW TEMPERATURE
      IF(T(M).LE.10.0) R(I,L)=R(I,L)*ALOG10(T(M))/4.0
C     CORRECT RATE FOR LOW MOISTURES
      IF(V(I).GE.10.0) R(I,L)=R(I,L)/ALOG10(V(I))*0.3
      IF(R(I,L)) 815,816,817
  815 IF(AMT(I,4).LT.ABS(R(I,L))) R(I,L)=-AMT(I,4)
      GO TO 816
  817 IF(AMT(I,3).LT.R(I,L))R(I,L)=AMT(I,3)
C     ADJUST  RATE FOR LENGTH OF TIME INTERVAL
  816 R(I,L)=R(I,L)/DELT
      DO 100 II=1,4
      C(II)=CC(II)
      B1(II)=BB1(II)
      B2(II)=BB2(II)
      B3(II)=BB3(II)
  100 CONTINUE
      RETURN
      END
```

```
C     SUBROUTINE FOR CALCULATING AVERAGE QUALITY OF RETURN FLOW
      SUBROUTINE AVQLTY
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BO,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,DAMT(2,5),DRN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      COMMON/BLK3/PCA(24,5),PCL(24,5),PHCO3(24,5),PMG(24,5),PNA(24,5),
     1PNO3(24,5),PSO4(24,5),OBJ,CCA(70),CMG(70),CNA(70),CCL(70),
     2CHCO3(70),CSO4(70),CCNO3(70)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      XNN=0.
      NLOW=1
      DO 5500 I=1,NMO
C     NUMBER OF PORE VOLUMES OF SUBSURFACE FLOW IN MONTH I=XNN
      XNN=XNN+XM*SUBSRF(I)/PV
      IF(XNN.LT..50) GO TO 5535
      XNN=XNN+.5
      NNN=XNN
      IF(LL.LE.NNN) TYPE 5009,NNN,LL,I
 5009 FORMAT(//10H**DANGER  ,2X,4HNNN=,I3,3X,3HLL=,I3,3X6HMONTH=,I3)
      IF(LL.LE.NNN) NNN=LL
      BCA=0.
      BMG=0.
      BNA=0.
      BSO4=0.
      BCL=0.
      BHCO3=0.
      BNO3=0.
      XJ=0.
      DO 5400 J=NLOW,NNN
C     COMPUTE TOTAL CONS ME/L
      BCA=BCA+CCA(J)
      BNA=BNA+CNA(J)
      BMG=BMG+CMG(J)
      BSO4=BSO4+CSO4(J)
      BCL=BCL+CCL(J)
      BHCO3=BHCO3+CHCO3(J)
      BNO3=BNO3+CCNO3(J)
 5400 XJ=XJ+1.
C     STORE AVERAGE CONC I=MONTH  NN=NUMBER OF SOIL TYPE
      PCA(I,NN)=BCA/XJ
      PMG(I,NN)=BMG/XJ
      PNA(I,NN)=BNA/XJ
      PSO4(I,NN)=BSO4/XJ
      PCL(I,NN)=BCL/XJ
      PHCO3(I,NN)=BHCO3/XJ
      PNO3(I,NN)=BNO3/XJ
      GO TO 5524
 5535 PCA(I,NN)=0.
      PMG(I,NN)=0.
      PNA(I,NN)=0.
      PCL(I,NN)=0.
      PSO4(I,NN)=0.
      PHCO3(I,NN)=0.
      PNO3(I,NN)=0.
C     COMPUTE TDS IN MG/L
 5524 TTDS=PCA(I,NN)/0.0499+PMG(I,NN)/0.08226+PNA(I,NN)/0.0435+
     1PSO4(I,NN)/0.02082+PCL(I,NN)/0.0282+PHCO3(I,NN)/0.01639+
     2PNO3(I,NN)/0.01612
      WRITE(6,5006) I,PCA(I,NN),PMG(I,NN),PNA(I,NN),PSO4(I,NN),
     1PCL(I,NN),PHCO3(I,NN),PNO3(I,NN),TTDS,NN
 5006 FORMAT(I3,7F8.2,F8.0,I6)
      IF(XNN.LT..50) GO TO 5500
      NLOW=NNN
      XNN=XNN-.5
 5500 CONTINUE
      RETURN
      END
```

```
C     SUBROUTINE TO COMPUTE SALTFLOW
      SUBROUTINE SALT
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSD(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
      COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
     1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
     2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
     3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
     4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
     5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
     6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
      COMMON/BLK3/PCA(24,5),PCL(24,5),PHCO3(24,5),PMG(24,5),PNA(24,5),
     1PNO3(24,5),PSO4(24,5),OBJ,DDCA(70),DMG(70),DNA(70),DCL(70),
     2DHCO3(70),DSO4(70),DNO3(70)
      COMMON/BLK4/AK(24),AMG(24),ANA(24),CA(24),CL(24),DAL(24),DP(24),
     1GWBF(24),HCO3(24),SMC,SMCH(24),SNPC(24),SO4(24),SPC,SRF(24),
     2STRC1(24),SUBSRF(24),SUMOUT(24),X1(24),X3(24)
      DO 3006 I=1,NMO
      DDCA(I)=0.
      DMG(I)=0.
      DNA(I)=0.
      DSO4(I)=0.
      DCL(I)=0.
      DHCO3(I)=0.
      DNO3(I)=0.
      DO 3005 NN=1,NS
      DDCA(I)=DDCA(I)+CO(NN)*PCA(I,NN)
      DMG(I)=DMG(I)+CO(NN)*PMG(I,NN)
      DNA(I)=DNA(I)+CO(NN)*PNA(I,NN)
      DSO4(I)=DSO4(I)+CO(NN)*PSO4(I,NN)
      DCL(I)=DCL(I)+CO(NN)*PCL(I,NN)
      DNO3(I)=DNO3(I)+CO(NN)*PNO3(I,NN)
 3005 DHCO3(I)=DHCO3(I)+CO(NN)*PHCO3(I,NN)
C     CORRECT CONCENTRATION OF NO3 TO BIOMASS UPTAKE
      DNO3(I)=DNO3(I)*UBIOM(I)
 3006 CONTINUE
      WRITE(6,5772)
 5772 FORMAT(///33H QUANTITY OF SURFACE OUTFLOW,TONS/)
      WRITE(6,5110)
 5110 FORMAT(/6H MONTH,5H   CA,6X,2HMG,6X,2HNA,6X,3HSO4,6X,2HCL,4X,
     14HHCO3,6X,3HNO3,6X,3HTDS/)
C     CALCULATE QUALITY OF COMBINED EFFLUENT
      SUMC=0.
      SUMM=0.
      YSQR1=0.
      DX=0.
      DY=0.
      DO 5600 J=1,NMO
C     CONVERT MOLES/L TO ME/L
      CA(J)=CA(J)*CF2
      AMG(J)=AMG(J)*CF2
      SO4(J)=SO4(J)*CF2
      CL(J)=CL(J)*CF1
      HCO3(J)=HCO3(J)*CF1
      ANA(J)=ANA(J)*CF1
      CNO3(J)=CNO3(J)*CF1
C     OBSERVED SURFACE WATER QUALITY
   82 GCA=CA(J)
      GMG=AMG(J)
      GSO4=SO4(J)
      GCL=CL(J)
      GNA=ANA(J)
      GHCO3=HCO3(J)
      GNO3=CNO3(J)
C     COMPUTED OUTFLOW CONCENTRATIONS
   84 CXA=SUBSRF(J)
C     ASSUME THAT CONC OF GWBF = CONC OF SURFACE INFLOW
      CXB=GWBF(J)
      CXC=STRC1(J)+SNPC(J)+SRF(J)
      CXD=SUMOUT(J)
      ECA=(CXA*DDCA(J)+CXB*GCA+CXC*GCA)/CXD
      EMG=(CXA*DMG(J)+CXB*GMG+CXC*GMG)/CXD
      ESO4=(CXA*DSO4(J)+CXB*GSO4+CXC*GSO4)/CXD
      ENA=(CXA*DNA(J)+CXB*GNA+CXC*GNA)/CXD
      EHCO3=(CXA*DHCO3(J)+CXB*GHCO3+CXC*GHCO3)/CXD
      ECL=(CXA*DCL(J)+CXB*GCL+CXC*GCL)/CXD
      ENO3=(CXA*DNO3(J)+CXB*GNO3+CXC*GNO3)/CXD
C     COMPUTED OUTFLOW OF IONS IN TONS
      U=.00227*CXD*ECA*AREA
      VV=.00138*CXD*EMG*AREA
      W=.00261*CXD*ENA*AREA
      X=.00544*CXD*ESO4*AREA
      Y=.00402*ECL*CXD*AREA
      Z=.00691*CXD*EHCO3*AREA
      ZN=0.00702*CXD*ENO3*AREA
      TT=U+VV+W+X+Y+Z+ZN
      TCOM(J)=TT
 5600 WRITE(6,5115) J,U,VV,W,X,Y,Z,ZN,TT
C     COMPUTE CORRELATION COEFFICIENT
      XNO=NMO
      DO 10 J=1,NMO
      SUMM=SUMM+X3(J)
   10 SUMC=SUMC+TCOM(J)
      XBAR=SUMM/XNO
      YBAR=SUMC/XNO
      DO 15 J=1,NMO
      DIFFX=X3(J)-XBAR
      DIFFY=TCOM(J)-YBAR
      YSQR=DIFFX*DIFFY
      DIFFX=DIFFX*DIFFX
      DIFFY=DIFFY*DIFFY
      DX=DX+DIFFX
      DY=DY+DIFFY
   15 YSQR1=YSQR1+YSQR
      YSQR1=YSQR1*YSQR1
      DNR=DX*DY
      RR=YSQR1/DNR
      R1=SQRT(RR)
      WRITE(6,1103) RR,R1,SUMM,SUMC
 5115 FORMAT(I3,7F8.0,F12.0)
 1103 FORMAT(/5H R*R=,F6.4,2X,3HR =,F6.4,2X,11HTOTALMEAS =,F10.0,
     12X,12HTOTAL CALC =,F10.0)
      RETURN
      END
```

```
C     SUBROUTINE TO COMPUTE EQUILIBRIUM CONCENTRATIONS
      SUBROUTINE XCHNGE(J,A,F,S,H,G,W,CASO,AGSO,XXT,B,SAT,
     1ET,TES,KK,CT,AN,ANH3,BNH4,DNH4)
      COMMON/BLK1/AREA,CF1,CF2,CO(5),D,DA,EC(20),ITX,L,LL,MM,NN,NS,PV,
     1TAGSO(20),TB(20),TC(20),TCA(20),TCASO(20),TCL(20),TCOM(20),TE(20),
     2THCO3(20),TK(20),TMG(20),TNA(20),TNO3(20),TSO(20),TSO4(20),
     3TXX(20),XLIME(20),XM,ZE(20)
C     GYPSUM REACTIONS= EQUIL CONC OF CA-SO4  EQN 19
   24 A1=A
      KC1=0
      KC2=0
      KC3=0
      IF(XXT) 4,4,26
    4 U=SQRT(2.*(A+F+G)+.5*(S+H+W+AN))
      AA=EXP(-9.366*U/(1.+U))
      IF(2.4E-5-A*G*AA) 26,18,18
   26 X=0.
      U=SQRT(2.*(A+F+G)+.5*(S+H+W+AN))
      BB=A+G
      EX=(9.366*U/(1.+U))
      CC=A*G-(2.4E-5)*EXP(EX)
      R=SQRT(BB*BB-4.*CC)
      X=(-BB+R)/2.
C     QTY OF ADDL ION PAIR THAT SHOULD BE PRESENT IN SAT GYPSUM SOLN
      CAS1=4.897E-3-CASO
      DEL=B*XXT-CAS1
      IF(DEL-X) 27,28,28
   27 X=XXT*B
      XXT=0.
      CAS1=0.
      A=A+X
      G=G+X
      U=SQRT(2.*(A+F+G)+.5*(S+H+W+AN))
C     UNDISSOCIATED (CA) (SO4) SOLVE EQN 22
      AA=EXP(-9.366*U/(1.+U))
    7 BB=-(4.9E-3+AA*A+AA*G)
      CC=AA*A*G-4.9E-3*CASO
      XXXX=BB*BB-4.0*AA*CC
      IF(XXXX) 35,35,36
   35 X1=0.
      GO TO 37
   36 X1=(-BB-SQRT(XXXX))/(2.*AA)
   37 CASO=CASO+X1
      A=A-X1
      G=G-X1
      GO TO 44
   18 IF(G) 1,1,6
    6 IF(A) 1,1,7
    1 IF(CASO) 44,44,7
   28 A=A+X
      G=G+X
      XXT=XXT-X/B
      CASO=CASO+CAS1
      XXT=XXT-CAS1/B
   44 A2=A
C     CA -NA EXCHANGE REACTIONS(SOLVE EQN 25)
      IF(S) 80,181,80
  181 IF(SAT) 80,515,80
   80 IJ=2
  404 IF(SAT-ET) 402,403,403
  402 Z=SAT/10.
      Z1=Z
```

```
      GO TO 5
  403 Z=ET/10.
      Z1=Z
    5 EX=EXP(-2.341*U/(1.+U))
      AA=-4.*DA*DA*B*B
      BB=4.*B*(EX+2.*DA*DA*ET*B+DA*DA*S)
      CC=4.*EX*(A+SAT*B)-4.*DA*DA*B*ET*(B*ET+2.*S)-DA*DA*S*S
      DD=SAT*EX*(4.*A+SAT*B)+2.*DA*DA*ET*S*(2.*B*ET+S)
      EE=SAT*SAT*A*EX-DA*DA*S*S*ET*ET
   81 ZZ=-((((AA*Z+BB)*Z+ CC)*Z+DD)*Z+EE)
      ZZZ=(((4.*AA*Z+3.*BB)*Z+2.*CC)*Z+DD)
      ZZ=ZZ/ZZZ
      IF(ZZ-0.0) 302,303,302
  303 IF(Z-0.0) 302,515,302
  302 ZZZ=ZZ/Z
      Z=Z+ZZ
      KC1=KC1+1
      IF(KC1.GT.50) TYPE 505
  505 FORMAT(//8HKC1 = 50//)
      IF(ABS(ZZZ)-.001) 83,83,81
   83 IF(Z.GE.0.0) GO TO 305
      IF(SAT.LT.ABS(Z*2.0)) Z=SAT/2.0
  305 A=A+B*Z
      IF(A) 510,510,512
  552 SAT=SAT-2.*Z
  551 ET=ET+Z
  550 S=S+2.*B*Z
  510 A=A-B*Z
      Z=-Z1
      GO TO 81
  512 S=S-2.*B*Z
      IF(S) 550,550,513
  513 ET=ET-Z
      IF(ET) 551,551,514
  514 SAT=SAT+2.*Z
      IF(SAT) 552,552,515
  515 A3=A
C     CA-MG EXCHANGE REACTIONS SOLVE EQN-24
      AA=B*(1.-D)
      BB=A+B*(CT+D*ET)+(D*F)
      CC=(A*CT-D*F*ET)
      R=SQRT(BB*BB-4.*AA*CC)
      Y=(-BB+R)/(2.*AA)
      A=A+B*Y
      F=F-B*Y
      ET=ET-Y
      CT=CT+Y
      A4=A
C     UNDISSOCIATED (MG)(SO4)  SOLVE EQN 22
      IF(G) 790,790,791
  791 IF(F) 790,790,792
  792 AA=EXP(-9.366*U/(1.+U))
      BB=-(5.9E-3+AA*F+AA*G)
      CC=AA*F*G-5.9E-3*AGSO
      XXXX=BB*BB-4.*AA*CC
      IF(XXXX) 793,793,794
  793 X1=0.
      GO TO 795
  794 X1=(-BB-SQRT(XXXX))/(2.*AA)
  795 AGSO=AGSO+X1
      F=F-X1
      G=G-X1
  790 CONTINUE
```

```
C       LIME REACTIONS
        GO TO (600,601),KK
  601   AA=4.
        BB=4.*(W+A)
        CC=W**2+4.*A*W
        DD=A*W**2-ZE(J)*EXP(2.341*U/(1.+U))
        IF(W-A) 61,61,62
   61   Z=-W/4.
        GO TO 650
   62   Z=-A/2.
  650   Z1=Z
   63   ZZ=-(((AA*Z+BB)*Z+CC)*Z+DD)
        ZZZ=((3.*AA*Z+2.*BB)*Z+CC)
        ZZ=ZZ/ZZZ
        Z=Z+ZZ
        KC2=KC2+1
        IF(KC2.GT.50) TYPE 506
  506   FORMAT(//8HKC2 = 50//)
        IF(ABS(ZZ).GT.1.E-5) GO TO 63
   64   A=A+Z
        W=W+2.*Z
        IF(W) 752,752,651
  752   W=W-2.*Z
        A=A-Z
        Z=-Z1
        GO TO 63
  651   IF(A) 752,752,753
  753   XLIME(J)=XLIME(J)-Z
  600   ZX=(A*W**2*EXP(-2.341*U/(1.+U)))
        IF(ZX.GE.ZE(J)) KK=2
        KC3=KC3+1
        IF(KC3.GT.100) TYPE 507,J
  507   FORMAT(//9HKC3 = 100,5X,4HJ  =,I2//)
        DEL=A-A1
C       A1= ORIGINAL CA
C       A2 = CA AFTER SOLVING EQNS 19 AND 22
C       A3 = CA AFTER SOLVING EQN 25
C       A4 = CA AFTER SOLVING EQN 24
        IF(ABS(DEL).GT.1.E-5) GO TO 24
        DEL=A-A2
        IF(ABS(DEL).GT.1.E-5) GO TO 24
        DEL=A-A3
        IF(ABS(DEL).GT.1.E-5) GO TO 24
        DEL=A-A4
        IF(ABS(DEL).GT.1.E-5) GO TO 24
        RETURN
        END
```

```
        SUBROUTINE RATE1(I,L,M)
        COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
       1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
       2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
       3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
       4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
       5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
       6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C       COMPUTE RATE OF UREA N HYDROLYSIS
  801   R(I,L)=C(L)+(B1(L)*ALOG10(T(M)))+(B2(L)*ALOG10(AMT(I,L)))
        IF(R(I,L).GE.-5.0) R(I,L)=-AMT(I,L)
C       CORRECT RATE FOR LOW TEMP
        IF(T(M).LE.10.0) R(I,L)=R(I,L)*ALOG10(T(M))/4.
C       ADJUST RATE FOR LENGTH OF TIME
  500   R(I,L)=R(I,L)/DELT
        RETURN
        END
```

```
        SUBROUTINE RATE2 (I,L,M)
        COMMON/BLK2/A,AACA(24),AAMT(2,4),AAMTRC(5),AAMTRN(5),AANO3(24),
       1AMT(5,5),AMTRC(5),AMTRN(5),AN,ANH3,AOR(24),AUREA(24),AACO3(24),
       2AASO4(24),AANH3(24),B1(5),B2(5),B3(5),BB1(4),BB2(4),BB3(4),BD,D1,
       3BNH4,C(5),CC(4),CCC,CN(5),CN1(5),CNO3(24),CNR,DELT,DELX,DNH4,ENH4,
       4FMCS,G,NMO,OAMT(2,5),ORN,P,PLNH4(24),PLNO3(24),R(5,5),RC(5),RN(5),
       5SM(24),SAMT(2,4),T(24),TEN(24),TNH3(24),TNH4(24),TTNH3(24),
       6TUREA(20),U1(24),UPTK(24),UREA,UBIOM(24),V(5)
C       COMPUTE RATE OF MINERALIZATION-IMMOBILIZATION
  751   R(I,L)=C(L)+(B1(L)*T(M))+(B2(L)*AMT(I,L))+(B3(L)*ALOG10(AMT(I,3)))
C       CORRECT RATE FOR LOW TEMP
        IF(T(M).LE.10.0) R(I,L)=R(I,L)*ALOG10(T(M))/4.0
C       CORRECT RATE FOR LOW MOISTURES
        IF(V(I).GE.10.0) R(I,L)=R(I,L)/ALOG10(V(I))*0.3
        IF(R(I,L).LT.0.0.AND.CN(I).GE.23.0) R(I,L)=0.0
        IF(R(I,L).LT.0.0.AND.CN(I).LT.23.0) R(I,L)=ABS(R(I,L))
C       CORRECT RATE FOR C/N RATIO
        R(I,L)=R(I,L)*(1.848*ALOG10(CN(I))-2.518)
        RETURN
        END
```

APPENDIX C

C. Definition of Variables

Input Variables

Mnemonic	Description	Units
ITY	OPVER option specification if ITY = 0 call QUAL = 1 simulation = 2 perform pattern search optimization. = 3 plot observed and simulated flows.	
VV_I	13 element vector of row headings for output tables, i.e. Jan, Feb, ... ANN.	
B_I	9 element vector of column headings for output tables, i.e. Alfa, Bean, ... Peas.	
PDL_K	Vector of proportion of daylight hours for months in the same order as vector VV.	
WKC_{IJ}	Array of crop use coefficients (in the same order as vector B) for crops for modified Blaney-Criddle equation. I is crop, J is month.	
DD_{jj}	JJ = 1 monthly surface inflow from canal diversions.	Acft
	= 2-5 monthly surface outflow from channels.	Acft
	= 6 monthly tributary inflow.	Acft
	= 7 monthly temperature	^oF
	= 8 monthly precipitation	inches

Mnemonic	Description	Units
NPH	Number of phases to be run during pattern search $1 \leq NPH \leq 5$	
NPR	Number of parameters 1 to 15	
XIN_L	Vector of initial parameters $L = 1$ to 14	
PL_L	Vector of lower bounds for parameters	
PM_L	Vector of upper founds for parameters	
NL_L	Vector of number of levels for each parameter	
$x1_I$	$I = 1$ Observed outflows Calcium	Tons
	$= 2$ " " Mg^{++}	Tons
	$= 3$ " " Na^{+}	Tons
	$= 4$ " " $SO^{=}_{4}$	Tons
	$= 5$ " " Cl^{-}	Tons
	$= 6$ " " HCO_3^{-}	Tons
	$= 7$ " " NO_3^{-}	Tons
C_I	Rate coefficients N-transformation equations	
$B1_I$	Rate coefficients N-transformation equations	
$B2_I$	Rate coefficients N-transformation equations	
$B3_I$	Rate coefficients N-transformation equations	
RN	Residual Nitrogen in soil layer	Percent
RC	Residual Carbon in soil layer	Percent
P_1	Porosity of soil layer 1	
D1	Depth of soil layer 1	cm
CNR_1	Initial carbon nitrogen ratio of soil layer 1	
DA	Equilibrium exchange constant Ca-Na	
D	Equilibrium exchange constant Ca-Mg	
TNH_4	Initial concentration of exchangeable NH_4^+ in soil layer	mol/gm
BD	Bulk density	gms/cm^3

Mnemonic	Description	Units
DELX	Depth of soil layer	cm
DELT	Time increment for nitrogen transformation rate equations	days
$AUREA_I$	Fertilizer application Urea in month I	lbs/Acre/month
$AANH3_I$	" " NH_3 "	"
$AANO3_I$	" " NO_3^- "	"
$AACA_I$	" " Ca^{++} "	"
$AACO3_I$	" " CO_3^- "	"
$AASO4_I$	" " $SO_4^=$ "	"
AOR_I	Organic matter application "	"
$UPTK_I$	Uptake of nitrogen by crops "	"
T_I	Temperature of soil layer 1 "	°F
TNO_3	Concentration of NO_3^- in solution (at pore volume saturation) in a soil layer	MEQ/L
TNH_3	Concentration of ammonium in soil solution in layer	"
TCA	Concentration of calcium in soil solution in layer	"
TMG	Concentration of magnesium in soil solution in layer	"
TNA	Concentration of sodium in soil solution in layer	"
TK	Concentration of potassium in soil solution in layer	"
$THCO_3$	Concentration of bicarbonate in soil solution in layer	"
TCL	Concentration of chloride in soil solution in layer	"
TSO_4	Concentration of sulphate in soil solution in layer	"
EC	Cation exchange capacity	MEQ/100 gms

Mnemonic	Description	Units
TE	Exchangeable Ca^{++} in soil layer	moles/gm
TC	" Mg^{++} "	"
TSO	" Na^{+} "	"
TXX	Gypsum in soil layer	"
XLIME	Lime content in soil layer	"
TB	Grams of soil/litre of soil solution	gms/liter
TCASO	Concentration of undissociated gypsum in soil layer	mol/liter
TUREA	Concentration of urea in soil layer	"
TAGSO	Concentration of undissociated $MgSO_4$ in soil layer	"
TEN	Soil moisture tension	bars
AOR_I	Application of organic matter in month I	lbs/acre
DNH_4	Equilibrium exchange constant Na-NH_4	
CCC	Conversion factor from lbs/acre to ug/sqcm	
$UBIOM_I$	Fractional uptake of nitrogen by biomass in month I	
NMO	Number of months of record	
NS	Number of different soils modeled	
ITX	Control option to print some additional output	
III	Control option to read common data from HYDSM	
CO(I)	Portion of irrigated area composed of soil I	
MM	Number of soil layers	
PV	Pore volume of soil	inches

Output Variables

Mnemonic	Description	Units
I	Month number	
EVT	Evapotranspiration by irrigated crops	inches
SM	Soil moisture content end of month I	inches
DP(I)	Deep percolation month I	inches[1]
SUMOUT	Total calculated surface water outflow month I	inches[1]
QMEASI	Total measured surface water outflow month I	inches[1]
DIFF	QMEASI minus SUMOUT	inches[1]
SRF(I)	Surface return flow	inches[1]
SUBSRF	Subsurface return flow	inches[1]
GWBF (I)	Correlated groundwater flow	inches[1]
SNPC(I)	Ungaged flow correlated with snowmelt	inches[1]
STRC1	Ungaged flow correlated with stream flow	inches[1]
RR	R squared	
RR, R_1	Correlation coefficient	
SUMM	Total measured water or salt outflow for model period	ac-ft or tons
SUMC	Total calculated water or salt outflow for model period	ac-ft or tons
PCA(I, NN)	Average concentration of Ca^{++} in effluent from soil NN for month I	meq/L
PMG(I, NN)	Average concentration of Mg^{++} in effluent from soil NN for month I	meq/L
PNA(I, NN)	Average concentration of Na^{+} in effluent from soil NN for month I	meq/L
PSO4(I, NN)	Average concentration of $SO_4^{=}$ in effluent from soil NN for month I	meq/L

Mnemonic	Description	Units
PCL(I, NN)	Average concentration of Cl^- in effluent from soil NN for month I	meq/L
PHCO3(I, NN)	Average concentration of HCO_3^- in effluent from soil NN for month I	meq/L
PNO3(I, NN)	Average concentration of NO_3^- in effluent from soil NN for month I	meq/L
TTDS	Total salt concentration in effluent from soil NN for month I	PPM
U	Computed total Ca^{++} outflow month I	tons
VV	Computed total Mg^{++} outflow month I	tons
W	Computed total Na^+ outflow month I	tons
X	Computed total $SO_4^=$ outflow month I	tons
Y	Computed total Cl^- outflow month I	tons
Z	Computed total HCO_3^- outflow month I	tons
ZN	Computed total NO_3^- outflow month I	tons
TT	Computed total salt outflow month I	tons

---

[1] equivalent inches over irrigated model area

APPENDIX D

```
 OCT   NOV   DEC   JAN   FEB   MAR   APR   MAY   JUN   JUL   AUG   SEP   ANN
7.68  6.59  6.35  6.58  6.63  8.80  9.00 10.16 10.27 10.88  9.64  8.40
 ALFA   BEAN   SPGR   PAST   SUBT   CORN   FLGR   POTA   PEAS
1ALFA     90.  79.  65.  63.  74.  86.  99. 112. 119. 110. 105.  99.
2BEAN     25.  29.  29.  29.  29.  28.  22.  67. 111.  89.  75.  20.
3SPGR     22.  29.  29.  29.  29.  28.  74. 118. 127.  73.  40.  29.
4PAST     80.  74.  58.  55.  66.  81.  86. 102.  99.  93.  91.  87.
5SUBT    102.  29.  29.  29.  29.  28.  22.  58.  95. 106. 120. 111.
6CORN     99.  29.  29.  29.  29.  28.  22.  60.  73.  93. 106. 109.
7FLGR     99.  29.  29.  29.  29.  28.  22.  60.  73.  93. 106. 109.
8POTA     22.  29.  29.  29.  29.  28.  22.  30.  42.  88. 131. 134.
9PEAS     90.  79.  65.  63.  74.  86.  99. 112. 119. 110. 105.  99.
  37811.   35333.   24302.   21623.   21069.   15765.    8100.
   3997.    2130.  170130.
  .22224   .20768   .14284   .12709   .12384   .09266   .04761
  .02349   .01251
66.66 45.45 41.13 40.28 44.26 48.35 55.63 86.33104.70 94.79 90.31 74.77
 .00  6.00  8.00  -.12   .70 20.00  8.00  7.50  3.00   .20
 .95   .00   .01  8.00  4.50  1.00  1.00  1.00   .00   .01   .00   .01
 .00   .00  4.00
 .82   .90   .90   .95   .99   .99   .86   .95   .92   .97   .97   .88
 .23   .28   .35   .28   .35   .45   .45   .60   .33   .25   .20   .20
1 1969  84199.  35099.   7300.      0.      0.   4900. 124699. 224599. 196599.
       227299. 227599. 156699.
2 1969  14599.   9399.   9500.   8000.   7500.   8000.  12699.  13799.  14500.
        15699.  15500.  15799.
3 1969    600.    300.    400.   2000.   1200.    600.   3200.   3300.   3700.
         4000.   2600.   4900.
4 1969   8699.   7700.   7300.   5800.   4200.   3400.   2000.   3900.   6700.
         6500.   6100.  12000.
5 1969  11699.   7800.   6600.   3000.   2500.   2500.   7700.   3800.   9000.
         4300.   4800.   8899.
6 1969    210.    200.    190.    700.    700.    310.    920.    600.   1300.
          500.      0.      0.
7 1969     48.     37.     28.     31.     29.     35.     49.     59.     62.
           71.     71.     62.
8 1969     .39    1.50    1.70     .50     .67     .09     .22     .06    1.13
           .25     .00     .49
```

```
 1 1970  63899.  30099.  11899.     100.     100.    6700.   79799. 193899. 193899.
        228500. 230599. 144000.
 2 1970  13199.    9799.  10500.    6800.    8199.    6500.    7800.   18199.  13000.
         13500.   15000.  17299.
 3 1970   4500.    2300.   2500.    1400.    1100.    1400.    5100.    5200.   5600.
          2800.    2700.   4500.
 4 1970  10299.    8500.   6300.    3800.    3800.    2800.    3000.    2800.   5800.
          6000.    6600.   9399.
 5 1970  12000.   11000.   9299.    1400.    1100.    1100.    6900.    5500.   8000.
          4000.    4500.  14699.
 6 1970      0.     300.    270.       0.       0.       0.       0.       0.      0.
             0.       0.      0.
 7 1970     44.      38.     32.      33.      38.      39.      41.      55.     64.
            72.      72.     55.
 8 1970     .52      .60    1.25     3.22      .27      .85      .89     1.08    1.67
            .44      .09     .78
OBSERVED SURFACE OUTFLOW IN TONS

 1     3768.2    1387.0    2977.6    5389.7    2054.3   15756.0      209.1

 2     2456.7     839.4    2278.1    4273.5    1578.7   12180.0      269.2

 3     2809.5    1077.2    2487.5    5223.5    1837.2   12396.0      228.0

 4     2577.6     866.5    2172.0    4131.2    1294.3   10013.0      171.3

 5     1663.0     713.0    1783.0    3121.0     962.0    7880.0      222.4

 6     1352.0     645.0    1541.0    2895.0    1175.0    7883.0       93.8

 7     1918.5     598.3    1878.3    2730.2    1269.3   13117.0       76.9

 8     2291.3     931.1    1933.2    2678.0    1216.2   11651.0       74.7

 9     3215.5     939.2    2332.5    3473.5    1629.5   16203.0      179.1

10     3165.5    1234.7    2454.3    3258.0    2132.1   12865.0      238.5

11     2705.0    1803.0    2308.6    3060.5    1805.3   16544.0      207.3

12     4098.7    2123.0    3682.0    4397.5    2054.0   19620.0      215.0
```

```
13    4016.1    1560.0    2928.3    2832.6    1535.5   18395.8     214.0

14    3615.5    1405.5    2953.2    4742.0    1667.5   15505.3     213.9

15    2846.6    1244.0    2673.5    4199.0    1625.7   14632.1     223.0

16    1581.0     532.6    1226.8    1835.8     734.6    7111.0     104.2

17    1897.2     574.0    1445.7    2275.0     864.0    7926.7     147.4

18    1360.3     478.4    1199.7    1704.2     800.6    4822.2     106.5

19    2805.3     754.3    1494.3    2455.2    1183.2   10006.8     108.2

20    3516.0    1086.0    1592.5    3384.6     877.7   10522.8     112.9

21    3198.3    1297.0    1848.5    3852.2    1370.0   12088.5     101.3

22    2699.0     969.2    1894.8    3526.6    1246.7   11601.5     162.5

23    2932.1    1138.2    2163.6    3168.8    1319.5   12186.0     212.7

24    4670.0    1893.0    3353.0    5391.2    2075.6   18916.5     339.8

INFLOW SURFACE WATER CONCENTRATION-MOLS/L

MON      CA         MG         NA        SO4         CL       HCO3         K
       NO3        NH3

 1   .137E-02   .663E-03   .958E-03   .873E-03   .688E-03   .343E-02   .110E-03
     .784E-05   .000E+00
 2   .142E-02   .414E-03   .119E-02   .118E-02   .817E-03   .354E-02   .179E-03
     .853E-05   .000E+00
 3   .144E-02   .722E-03   .117E-02   .140E-02   .912E-03   .386E-02   .129E-03
     .214E-04   .000E+00
```

```
  4  .525E-03  .165E-03  .160E-03  .100E-02  .210E-03  .161E-02  .100E-03
     .215E-05  .000E+00
  5  .550E-03  .200E-03  .140E-03  .312E-03  .130E-03  .144E-02  .180E-03
     .285E-05  .000E+00
  6  .120E-02  .412E-03  .825E-03  .595E-03  .451E-03  .447E-02  .108E-03
     .730E-05  .000E+00
  7  .919E-03  .556E-03  .953E-03  .497E-03  .645E-03  .408E-02  .139E-02
     .361E-05  .000E+00
  8  .153E-02  .738E-03  .538E-03  .873E-03  .498E-03  .386E-02  .999E-04
     .107E-05  .000E+00
  9  .976E-03  .547E-03  .606E-03  .682E-03  .496E-03  .382E-02  .110E-03
     .712E-05  .000E+00
 10  .963E-03  .628E-03  .679E-03  .748E-03  .738E-03  .265E-02  .120E-03
     .178E-05  .000E+00
 11  .105E-02  .690E-03  .680E-03  .750E-03  .660E-03  .344E-02  .900E-04
     .178E-05  .000E+00
 12  .122E-02  .735E-03  .920E-03  .437E-03  .610E-03  .325E-02  .100E-03
     .178E-05  .000E+00
 13  .130E-02  .725E-03  .105E-02  .437E-03  .680E-03  .386E-02  .100E-03
     .714E-05  .000E+00
 14  .113E-02  .658E-03  .136E-02  .804E-03  .732E-03  .426E-02  .990E-04
     .198E-04  .000E+00
 15  .149E-02  .811E-03  .117E-02  .825E-03  .840E-03  .409E-02  .176E-03
     .296E-04  .000E+00
 16  .142E-02  .775E-03  .118E-02  .750E-03  .750E-03  .425E-02  .160E-03
     .228E-04  .000E+00
 17  .105E-02  .700E-03  .118E-02  .687E-03  .700E-03  .452E-02  .160E-03
     .535E-05  .000E+00
 18  .150E-02  .725E-03  .150E-02  .500E-03  .890E-03  .343E-02  .240E-03
     .714E-05  .000E+00
 19  .142E-02  .525E-03  .100E-02  .437E-03  .830E-03  .397E-02  .140E-03
     .000E+00  .000E+00
 20  .142E-02  .625E-03  .850E-03  .500E-03  .480E-03  .338E-02  .120E-03
     .000E+00  .000E+00
 21  .137E-02  .725E-03  .710E-03  .562E-03  .580E-03  .304E-02  .100E-03
     .178E-05  .000E+00
 22  .130E-02  .725E-03  .610E-03  .437E-03  .490E-03  .301E-02  .110E-03
     .392E-05  .000E+00
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 23  .122E-02  .600E-03  .680E-03  .376E-03  .400E-03  .298E-02  .110E-03
     .392E-05  .000E+00
 24  .100E-02  .700E-03  .740E-03  .375E-03  .400E-03  .307E-02  .100E-03
     .000E+00  .000E+00
  8.00  7.98 49.999999.99 10.00  3.00   .70  1.30152.00   .22   .033
                                                                     PLNO3     PLNH4
MO ANH4   AANO3  AUREA  AACA   AACO3  AASO4   AOR    UPTK    T   UBOIM
 1  4.000   .000  3.500   .000   .000   .000170.364 62.000  9.500   .400  .1021E+00 .5377E-02
 2   .000   .000   .000   .000   .000   .000    .000 43.000  9.500   .500  .7086E-01 .3729E-02
 3   .000   .000   .000   .000   .000   .000    .000 38.000  7.000   .450  .6262E-01 .3296E-02
 4   .000   .000   .000   .000   .000   .000    .000 37.000  8.000   .550  .5984E-01 .3149E-02
 5   .000   .000   .000   .000   .000   .000    .000 41.000  7.500   .750  .6515E-01 .3429E-02
 6  9.000   .000 16.500   .000   .000   .000  56.788 45.000  6.500   .400  .7393E-01 .3891E-02
 7  9.000   .000 16.500   .000   .000   .000  56.788 52.000  9.000   .500  .8543E-01 .4496E-02
 8  9.000   .000 16.500   .000   .000   .000  56.788 82.000 11.000   .250  .1346E+00 .7088E-02
 9  7.000   .000 13.500   .000   .000   .000    .000 98.000 16.000   .500  .1609E+00 .8471E-02
10   .000   .000   .000   .000   .000   .000    .000 87.000 17.000   .500  .1429E+00 .7525E-02
11   .000   .000   .000   .000   .000   .000  56.788 84.000 17.000   .500  .1379E+00 .7261E-02
12  4.000   .000  3.500   .000   .000   .000170.364 70.000 14.000   .500  .1149E+00 .6051E-02
13  4.000   .000  3.500   .000   .000   .000170.364 62.000  9.500   .440  .1018E+00 .5361E-02
14   .000   .000   .000   .000   .000   .000    .000 43.000  9.500   .490  .7065E-01 .3718E-02
15   .000   .000   .000   .000   .000   .000    .000 38.000  7.000   .390  .6241E-01 .3285E-02
16   .000   .000   .000   .000   .000   .000    .000 37.000  8.000   .500  .6081E-01 .3200E-02
17   .000   .000   .000   .000   .000   .000    .000 41.000  7.500   .570  .6631E-01 .3490E-02
18  9.000   .000 16.500   .000   .000   .000  56.788 45.000  6.500   .360  .7391E-01 .3890E-02
                                                                          .8546E-01 .4498E-02
                                                                          .1347E+00 .7093E-02
                                                                          .1610E+00 .8477E-02
19  9.000   .000 16.500   .000   .000   .000  56.788 52.000  9.000   .600  .1429E+00 .7523E-02
20  9.000   .000 16.500   .000   .000   .000  56.788 82.000 11.000   .270  .1380E+00 .7266E-02
21  7.000   .000 13.500   .000   .000   .000    .000 98.000 16.000   .490  .1150E+00 .6055E-02
22   .000   .000   .000   .000   .000   .000    .000 87.000 17.000   .490
23   .000   .000   .000   .000   .000   .000  56.788 84.000 17.000   .490
24  4.000   .000  3.500   .000   .000   .000170.364 70.000 14.000   .560
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CONCENTRATIONS OF INITIAL SOIL SOLUTION

   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00


   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00


   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00


   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00


   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00


   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00




   .1500E+01 .1200E+01 .1000E+02 .1100E+00 .1400E+01 .1500E+01 .1000E+02
   .1250E+02 .7000E+01 .3150E+01 .6000E-01 .0000E+00 .0000E+00 .2500E+00
   .3000E-01 .0000E+00
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APPENDIX E

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YR MO SRF  SUBSRF EVT   GWBF  SNPC  STRC SMCH    DAL   DP  SUMOUT QMEAS DIFF
 1  1    .91  1.37  1.26  -.00  -.01   .06  3.21  4.08  3.20  2.33  2.10   .22
 1  2    .22  1.20   .36  -.00   .01   .03  3.00  1.86  2.99  1.46  1.49   .02
 1  3    .06  1.36   .11  -.00  -.01   .01  1.97   .39   .26  1.43  1.40   .02
 1  4    .01   .89   .18  -.00  -.01   .01   .34   .02  -.01   .91  1.11   .19
 1  5    .01   .77   .16  -.00  -.01   .01   .53   .02  -.01   .79   .91   .11
 1  6    .02   .55   .45  -.00   .01   .01  1.00   .29   .99   .60   .85   .25
 1  7   1.05   .32  1.30  -.00   .01   .09  6.86  6.38  6.87  1.47  1.51   .03
 1  8    .67   .76  3.78  -.00  -.01   .14  9.15 12.65  9.14  1.57  1.46   .10
 1  9    .94   .98  5.23  -.00  -.00   .13  6.66 10.76  6.66  2.05  2.00   .05
 1 10    .41  1.24  6.86  -.00  -.01   .14  6.46 13.06  6.45  1.79  1.80   .01
 1 11    .41  1.28  3.81   .01  -.01   .14  7.24 13.05  7.23  1.85  1.71   .13
 1 12   1.12  1.41  3.05  -.00  -.01   .10  5.58  8.14  5.57  2.63  2.46   .17
   18.867  18.952    -.085
 2  1    .69  1.60  1.01  -.00  -.01   .04  2.59  3.09  2.58  2.33  2.36   .03
 2  2    .20  1.72   .40   .01  -.01   .03  1.79  1.60  1.79  1.96  1.87   .09
 2  3    .08  1.69   .20  -.00   .00   .02  1.68   .63  1.67  1.81  1.69   .11
 2  4    .01   .98   .22  -.00   .01   .01  2.98  -.01  2.98  1.03   .79   .24
 2  5    .01   .89   .39  -.00  -.01   .01  -.14  -.01  -.01   .91   .84   .07
 2  6    .02   .86   .58   .01  -.01   .01   .65   .38   .63   .91   .69   .21
 2  7    .67   .67   .83   .01  -.01   .06  4.09  4.04  4.09  1.41  1.34   .06
 2  8    .58   .97  3.07   .01  -.01   .12  8.89 10.89  8.88  1.69  1.87   .17
 2  9    .93   .88  5.63  -.00   .01   .12  6.58 10.55  6.57  1.94  1.91   .03
 2 10    .41  1.08  6.96   .01  -.01   .14  6.58 13.11  6.56  1.65  1.55   .09
 2 11    .42  1.15  5.88   .01  -.01   .15  7.43 13.22  7.43  1.73  1.70   .03
 2 12   1.03  1.33  2.19   .01  -.01   .09  6.06  7.48  6.06  2.47  2.71   .24
   19.388  19.900    -.512

R*R= .9344  R= .9666  TOTAL MEAS=  646199.  TOTAL CALC=  656292.
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QUALITY OF PERCOLATED EFFLUENT IN ME/L TDS IN MG/L

MONTH	CA	MG	NA	SO4	CL	HCO3	NO3	TDS	SOIL
1	3.19	2.61	3.00	1.96	1.40	6.52	.25	722.	1
2	3.19	2.61	3.00	1.96	1.40	6.52	.25	722.	1
3	3.19	2.61	3.01	1.88	1.39	6.52	.25	718.	1
4	3.20	2.61	3.01	1.80	1.39	6.51	.25	714.	1
5	3.20	2.62	3.01	1.73	1.39	6.50	.25	711.	1
6	3.20	2.62	3.02	1.65	1.39	6.50	.25	707.	1
7	3.20	2.62	3.02	1.65	1.39	6.50	.25	707.	1
8	3.21	2.62	3.02	1.58	1.39	6.49	.25	703.	1
9	3.21	2.62	3.02	1.52	1.39	6.49	.25	700.	1
10	3.21	2.62	3.02	1.47	1.39	6.49	.25	698.	1
11	3.21	2.63	3.02	1.42	1.39	6.48	.25	695.	1
12	3.21	2.63	3.02	1.39	1.39	6.48	.25	694.	1
13	3.21	2.62	3.02	1.34	1.38	6.48	.25	691.	1
14	3.20	2.62	3.02	1.31	1.36	6.49	.25	689.	1
15	3.19	2.61	3.02	1.30	1.34	6.50	.24	688.	1
16	3.18	2.60	3.01	1.30	1.33	6.51	.24	687.	1
17	3.17	2.59	3.01	1.30	1.31	6.52	.24	686.	1
18	3.16	2.58	3.00	1.30	1.29	6.53	.24	686.	1
19	3.16	2.58	3.00	1.30	1.29	6.53	.24	686.	1
20	3.14	2.57	2.99	1.30	1.27	6.55	.23	685.	1
21	3.13	2.56	2.99	1.30	1.25	6.56	.23	685.	1
22	3.11	2.54	2.98	1.30	1.23	6.58	.22	684.	1
23	3.09	2.53	2.97	1.30	1.21	6.60	.22	683.	1
24	3.07	2.51	2.96	1.30	1.18	6.62	.21	682.	1

```
QUALITY OF PERCOLATED EFFLUENT IN ME/L TDS IN MG/L

MONTH  CA      MG      NA      SO4      CL     HCO3      NO3     TDS      SOIL

  1   4.78    3.92    3.78    3.15    1.40    7.83      .25    925.      2
  2   4.78    3.92    3.78    3.15    1.40    7.83      .25    925.      2
  3   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  4   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  5   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  6   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  7   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  8   4.77    3.92    3.78    3.15    1.39    7.83      .25    925.      2
  9   4.77    3.91    3.78    3.15    1.39    7.83      .25    925.      2
 10   4.77    3.91    3.78    3.14    1.39    7.83      .25    924.      2
 11   4.76    3.91    3.78    3.14    1.39    7.84      .25    924.      2
 12   4.76    3.90    3.78    3.13    1.39    7.84      .25    924.      2
 13   4.74    3.89    3.77    3.11    1.38    7.85      .25    923.      2
 14   4.71    3.87    3.76    3.07    1.36    7.87      .25    921.      2
 15   4.67    3.84    3.75    3.02    1.34    7.90      .25    917.      2
 16   4.65    3.82    3.74    2.99    1.33    7.92      .25    916.      2
 17   4.62    3.79    3.73    2.95    1.31    7.95      .24    913.      2
 18   4.59    3.76    3.72    2.91    1.29    7.97      .24    911.      2
 19   4.59    3.76    3.72    2.91    1.29    7.97      .24    911.      2
 20   4.55    3.73    3.70    2.86    1.27    8.00      .24    908.      2
 21   4.51    3.70    3.69    2.81    1.25    8.03      .23    905.      2
 22   4.46    3.66    3.67    2.74    1.23    8.07      .23    901.      2
 23   4.42    3.63    3.66    2.68    1.21    8.11      .23    898.      2
 24   4.37    3.59    3.64    2.62    1.18    8.15      .22    894.      2
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QUANTITY OF SURFACE OUTFLOW,TONS

MONTH    CA       MG        NA        SO4        CL     HCO3          NO3        TDS

  1    3731.    1611.    2950.     5729.     2104.   18416.       205.        34748.
  2    2549.    1160.    2324.     4080.     1546.   13390.       216.        25267.
  3    2603.    1286.    2504.     4019.     1612.   14132.       221.        26372.
  4    1656.     822.    1615.     2503.     1026.    9059.       175.        16860.
  5    1433.     711.    1397.     2101.      886.    7825.       207.        14562.
  6    1076.     522.    1026.     1540.      653.    5892.        80.        10792.
  7    1575.     658.    1171.     2130.      978.    9867.        64.        16446.
  8    2547.    1034.    1607.     3561.     1199.   12060.        69.        22080.
  9    2771.    1228.    2116.     4150.     1553.   15617.       186.        27625.
 10    2782.    1336.    2449.     4090.     1751.   14577.       224.        27212.
 11    2908.    1395.    2522.     4176.     1765.   15631.       231.        28631.
 12    3967.    1795.    3142.     4710.     2210.   19756.       256.        35840.
 13    3812.    1760.    3293.     4648.     2211.   20070.       260.        36056.
 14    3393.    1655.    3272.     4604.     2064.   18788.       309.        34088.
 15    3233.    1585.    3115.     4264.     1940.   17804.       240.        32182.
 16    1842.     907.    1793.     2416.     1100.   10260.       176.        18496.


 17    1630.     810.    1614.     2138.      974.    9232.       179.        16580.
 18    1615.     792.    1584.     2072.      954.    9059.       109.        16186.
 19    2172.     817.    1593.     2282.     1215.   10977.       140.        19199.
 20    2670.    1112.    2051.     3033.     1297.   13348.        89.        23603.
 21    2901.    1209.    1969.     3331.     1412.   13604.       149.        24578.
 22    2569.    1172.    2094.     2971.     1317.   13520.       178.        23823.
 23    2650.    1191.    2238.     3028.     1329.   14333.       186.        24958.
 24    3332.    1564.    2776.     3829.     1658.   18702.       235.        32120.

R*R= .8145  R = .9024  TOTALMEAS =   568220.  TOTAL CALC =   588316.
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VITA

Visvanatha A. Narasimhan

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Doctor of Philosophy

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Major Field: Civil and Environmental Engineering

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Professional Experience: 1975, Research Engineer, Utah Water Research Laboratory, Logan, Utah. 1971-1974, Graduate Research Assistant, Utah Water Research Laboratory, Logan, Utah. 1969-71, Executive Engineer, Food Storage Division, Karnal (Haryana), India; 1965-68, Assistant Engineer Designs, Sonauli Pokhara Road Project, Butwal, Nepal (a Govt. of India Assignment in the AID project); 1961-65, Assistant Engineer, Designs, Central Public Works Department, New Delhi, India; 1957-60, Design and Engineering Assistant, Central Water and Power Commission, New Delhi, India.

Professional Activities: Indian Roads Congress, Institution of Structural Engineers (London) and American Water Resources Association.

Honors and Awards: Who's Who among the heads of Construction Divisions for outstanding performance in Central Public Works Department, New Delhi, India in 1970-71; Successful in the Combined Engineering Services Examination held by Union Public Service Commission, New Delhi, India in 1960; Recipient of Gonsalves medal for being first for the college in the Intermediate Examination in 1953. Recipient of prizes for outstanding performace in studies during many of the high school years, 1945-51.