Management-Oriented Modeling:
Optimizing Nitrogen Management using Computerized Artificial Intelligence

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in Partial Fulfillment of the Requirements for the Degree of
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in Agronomy and Soil Science

By

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We certify that we have read this dissertation and that, in our opinion, it is satisfactory in scope and quality as a dissertation for the degree of Doctor of Philosophy in Agronomy and Soil Science.

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To my happy family:

Zhufeng Zhang and Zhiding LI, my parents and
Xianyu Wen, my wife and my child Lee LI

Abstract

Increasing nitrate levels in groundwater have caused growing public health concern in recent years. This has prompted research on precision nitrogen management to understand and control nitrogen impact on the environment. Many nitrogen (N) models have been developed to describe the N status and behavior in soil-plant systems, but they are uniformly weak in finding optimal management strategies. To model nitrogen management, Management-Oriented Modeling (MOM), a dynamic simulation model using artificial intelligence (AI) optimization techniques, was developed in this study. MOM was designed as a tool to find optimal solutions for N management to minimize nitrate leaching and maximize production and profits.

MOM consists of a generator, a simulator, and an evaluator. In searching for optimal management strategies, the generator produces a group of nodes (management choices). The evaluator uses the built-in knowledge and communication with users to analyze the outputs of the simulator and to guide the generator's work. A mixed search method that combines *hill-climbing* method for a global, strategic search with *best-first* method for a local, tactical search was developed to find the shortest path from start nodes to goals. In this manner, MOM searches for user-weighted goals by simulating the N cycle and management effects on the fate of N in a soil-plant system. In addition to general simulation and evaluation of N fertilization, MOM provides real time decision-aid for within-season management. MOM-guided within-season management uses weather forecasting to estimate rainfall in the near future and

simulates the consequences in soil-plant systems. It gives users daily "snapshots" of the N status in soil-plant systems without within-season sampling and testing. Scenarios show that MOM can provide precision nitrogen management that maximizes profits and yields while minimizing nitrate leaching by updating management of irrigation and fertilization within-season. MOM-guided within-season management is a precision tool with high efficiency, low cost and "transparency" for nitrogen management. MOM simulator was evaluated with 11 datasets from Hawaii and Brazil. Calibration and validation results suggest that the model prediction accuracy was acceptable for the field N management.

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Preface

The emergence of artificial intelligence (AI) technologies have brought great changes to the world. In the past three to four decades, the artificial intelligence has been fully developed in many areas such as space, finance, communications and military. The theory of knowledge-based systems, an AI field, is about two decades old (Plant and Stone, 1991). However, the development of the artificial intelligence in agriculture had only began in the last decade. For example, *AI Applications*, first AI journal for natural resources, agriculture, and the environmental science, began publication in 1987. As a young field, AI applications in agriculture and the environment provide many opportunities for researchers who sense the challenge and opportunity the area offers. This study is an exploration in managing quantitative agricultural information with AI technologies. Many explorations in the dissertation remain unfinished. The dissertation is not an end but may be a beginning for Management-Oriented Modeling. I hope that the work presented in the dissertation will contribute a "brick" to the "building" of precision agriculture that is revolutionizing modern agriculture.

Federal Government Hatch Project F93-272-F-531-8-145, which has fully supported this study since 1992, is acknowledged. A special thanks is due Dr. Russell S. Yost. He is not only my major adviser, but also a major author of this dissertation. We have discussed my research of Ph. D. program weekly since 1992 and the discussion has been focused on the work presented in this dissertation since 1995. Many original ideas came from brainstorming during our discussions. For five years of my graduate study, Dr. Yost has supported me much more than academic advice. Under his excellent teaching, kind understanding, love to students, and influence of his life philosophy, I have been thoroughly enjoying my graduate program for years. I cannot express my thanks to his by words, let me cite Dr. Yost's philosophy for education as a gratefulness to him: encourage and assist students design their own unique pursuit of excellence, innovativeness, of creativity, and of enthusiasm to sciences, and cooperative learning, especially important in graduate education levels.

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University of Hawaii
Fall, 1997

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Chapter 1

Introduction

Nitrate levels in groundwater are a growing public health concern in recent years. Nitrogen (N) fertilizer applications in excess of crop N removals in agriculture is considered an important source of nitrate leaching from the root zone into groundwater. This has prompted research on nitrogen budgets in soil-crop systems and the development of nitrogen models addressing N impact on food production, economic profitability and environmental health (Bacon, 1995).

1-1. Nitrogen Impact on the Environment

Nitrogen is no doubt one of the most important plant nutrients and Number One fertilizer for crop production (Hauck, 1984). Global food production dramatically increased in the past two decades of the Green Revolution. Synthetic nitrogen fertilizer made a major contribution with the high-yield crop varieties to the Green Revolution. World cereal production rose approximately 50 percent from 1.2 billion metric tons in

1970 to about 1.8 billion metric tons in 1989 (Livernash, 1993). During the same period, inorganic nitrogen fertilizer consumption increased 267 percent from about 30 million metric tons to about 80 million metric tons (FAO, 1991). However, nitrate levels in groundwater have also been found to increase dramatically in the past decade. A contractor report prepared for the Office of Technology Assessment found at least 8,200 wells in vulnerable regions of the U.S. with nitrate concentration exceeding the Maximum Contamination Level (MCL) of 10 mg NO_3-N L^{-1}, which was established by the U.S. Environmental Protection Agency (EPA) to protect public health (U.S. Congress, 1990). It was estimated that about 25 percent of the population in the European Community (EC) was drinking water with a nitrate nitrogen level greater than the EC's recommended maximum level of 25 mg L^{-1} (Gardner, 1990). A survey from 14 cities and counties (covered 120,000 km^2) in North China found over half of 69 surveyed sites with nitrate levels in groundwater or drinking water exceeding 10 mg NO_3-N mg L^{-1}. Nitrate concentration of groundwater in some small towns in vegetable production areas was greater than 60 mg NO_3-N L^{-1} (Zhang *et al.*, 1994). In Hawaii, nitrate nitrogen concentrations have been found up to 7-8 mg L^{-1} in some Board of Water Supply wells at the central parts of Oahu (El-Kadi, 1996). This implies the aquifer that supplies 48% of the water used on Oahu will become unsuitable for our infants unless the increase stops. "The nitrate issue" has shifted in scale from a local pollution problem to public concern nationwide and across the world.

What negative impacts does nitrate impose on the environment? One of the impacts is eutrophication of water bodies. The algal bloom resulting from enrichment of surface water by nitrogen and phosphorus will disturb the ecological balance in freshwater and marine ecosystems. Drinking-water is also contaminated by algae because many algae are toxic to humans (Heathwaite *et al.*, 1993). The most important impact of nitrate on the environment, however, is its direct toxicity to humans. The lethal nitrate dose in human adults is 4 to 50 g of nitrate and 1.6 to 9.5 g of nitrite. A small amount of nitrate salts is not harmful directly. Its toxicity is because ingested nitrate can be reduced to nitrite (Mirvish, 1991). High concentration of nitrite can react with hemoglobin in the bloodstream to form methemoglobin. This causes a medical condition called methemoglobinemia (mostly in babies less than six months old), in which the ability of hemoglobin to carry oxygen is restricted and results in oxygen-starved or bluish-tinged baby ('blue-baby' syndrome). There were 320 cases of methemoglobinemia in infants drinking well water with high concentration nitrate in US from 1939 to 1950 (Walton, 1951), 745 cases in Germany from 1956 to 1960 (Mirvish, 1991), and 2,000 cases worldwide reported by WHO between 1945 and 1986 (Heathwaite *et al.*, 1993). Among these infants, 160 died as a result of drinking water with nitrate concentrations greater than 25 mg NO_3-N L^{-1} from unsterilized feeding bottles (Heathwaite *et al.*, 1993). Walton (1951) reported from a survey that infant methemoglobinemia occurred in 0%, 2.3%, and 17% of cases who drank water with nitrate nitrogen concentrations of less than 10, 10 to 20, and 20 to 40 mg L^{-1} respectively. This finding provided the basis for US EPA and WHO to establish the upper limit of 11.3 mg NO_3-N L^{-1} in drinking water (Mirvish, 1991). Some epidemiologic studies further indicate an association between nitrate and non-Hodgkin's lymphoma (HNL), stomach cancer, and possibly birth defects (National Coalition for Agricultural Safety and Health, 1989).

In addition to pesticides, nitrate has become a source of nonpoint pollution, and the most widespread nutrient contaminant in the past decade. In contrast to point source pollution, nitrate pollution of groundwater from nonpoint sources is difficult to eradicate by regular treatment technologies. Drinking water cleanup from agrochemical nonpoint source contamination is likely to be very costly, and may be technically infeasible if the concentration is low. A study of potential costs of groundwater contamination estimated that initial household monitoring alone would cost approximately $1.4 billion (Nielsen and Lee, 1987). If nitrate level in an aquifer reaches the EPA Maximum Contamination Level (MCL), the remedial actions of groundwater cleanup would impose a large burden on rural homeowners and small communities. The only choice may be closing wells. For example, Hawaii Department of Health shut down several public wells on Oahu in 1983, because the nematicides EDB, DBCP, and trichloropropane were detected (Lau and Mink, 1987). Some residents of central Oahu had to obtain drinking water from a tank truck. A public well was shut down and seven others were placed under monitoring in Honolulu in 1996 due to traces of termite poison found in the wells (Wright, 1996). Nonpoint pollution, including contamination by pesticides and nitrate, has been a challenge to not only communities and scientists, but also the whole society and political leaders.

U.S. Congress enacted several Acts regulating the contaminations associated with agricultural chemicals, for example, Coastal Zone Management Act of 1972, Safe

Drinking Water Act of 1974 and amended in 1986, Water Quality Act of 1987, and Coastal Zone Act Reauthorization Amendments of 1990 (CZARA). These Acts addressed several concerns. A major one was the impact of **nonpoint source** pollution on coastal water (EPA, 1993). Some statements in section 6202 (a) of CZARA are quoted below:

"1. Our oceans, coastal waters, and estuaries constitute a unique resource. The condition of the water quality in and around the coastal areas is significantly declining. Growing human pressures on the coastal ecosystem will continue to degrade this resource until adequate actions and policies are implemented.

. . . .

"5. Nonpoint source pollution is increasingly recognized as a significant factor in coastal water degradation. . . .

"6. Coastal planning and development control measures are essential to protect coastal water quality, which is subject to continued ongoing stresses. Currently, not enough is being done to manage and protect coastal resources."

To address more specifically the impacts of nonpoint source pollution on coastal water quality, Congress enacted section 6217 "Protecting Coastal Water," which was codified as 16 U.S.C. §1455b (EPA, 1993). This section provides that each State with an approved coastal zone management program must develop and submit to EPA for approval a Coastal Nonpoint Pollution Control Program. The purpose of the program "shall be to develop and implement management measures for nonpoint source pollution to restore and protect coastal waters, working in close conjunction with other State and local authorities." These acts reflected public concerns about possible groundwater contamination and changed goals of nitrogen management. Since the middle of 1970s, many nitrogen investigations have targeted improving nitrogen management in reducing nitrate leaching to groundwater (Smika *et al.*, 1977; Timmons and Dylla, 1981; Hergert, 1986; Follett *et al.*, 1991; Bacon, 1995). In the 1990s, a major agricultural theme has been shifted from increasing production and economic return to concern about environmental health while maintaining food production.

1-2. Modeling Approach to Solving N Problems

There have been two different approaches to study the real world: reductionism and systems methods. As a method of science, the reductionist approach has a history of hundreds of years, while the systems approach is an infant discipline, only about thirty years old (Checkland, 1989). With the reductionist approach, the complexity of the real world is reduced in controlled experiments and hypotheses are refuted to obtain knowledge. A common reductionist approach, hypothetic-deductive model of scientific justification, could be described as *Hypothesis* + *Experiments* = *Deduction* ⇒ *Conclusion* (Tiles, 1995). This is a typical analysis approach. In contrast to reductionism, the systems approach is a synthetic method "which takes a broad view, which tries to take all aspects into account, which concentrates on interactions between the different parts of the problem" (Checkland, 1989). Not focusing on a particular set of phenomena, a systems approach is a meta-discipline applied with many other disciplines where components interact with each other. Problems in agriculture and the environment need cooperative problem solving of multiple disciplines. The systems approach has become an important research method in the sciences of agriculture and the environment. For controlling contamination by nitrate leaching, involving many physical, chemical and biological processes, systems methods have been useful tools.

Computer decision aid systems are systems methods applied in agriculture and the environment. Some of these decision aid systems could be simply categorized as (1) Database Management Systems (DBMS), (2) Geographic Information System (GIS), (3) Simulation Models (SM), (4) Management Science / Operations Research (MS/OR), and (5) Expert Systems (ES). DBMS and GIS are information delivery tools which provide easy access to relevant information. SM rapidly simulates consequences of varying inputs to explore specific processes in the real world. DBMS, GIS and SM were not initially designed to solve problems but to effectively manipulate information. MS/OR and ES are often used for problem solving. A common MS/OR method is linear programming (LP) that provides optimal numerical solutions for problems (Anderson, *et al.* 1994). ES include knowledge-based systems that can capture 'knowledge' such as logical rules, experience, and qualitative information in addition to handling numerical information. Search and pattern matching techniques are broadly used in expert systems as the major problem-solving strategies.

In recent years, many nitrogen models have been developed using one or more of the techniques above. These models have been developed with many objectives and assumptions. Some are designed to record state-of-the-art knowledge while others are designed for ease of use and minimal data requirements. Table 1-2.1 lists some nitrogen models that have been developed since 1980.

These models addressed N problems in the estimation of N budget, dynamical simulation of the N cycle in soil-plant systems, environmental impact assessments, and general management recommendations. Many of these models consist of complex

Table 1-2.1. Some nitrogen models developed since 1980

Model	Authors	Application
AGNPS	Yong, *et al.*, 1989	Non-point source pollution evaluation for watersheds
CENTURY	Parton, *et al.*, 1988	Simulating the cycle of C, N, S, and P through organic matter
CERES-N	Ritchie, *et al.* 1986	Simulation of maize growth and development, N sub-model
CREAMS	Knisel, 1980	Chemical, runoff and erosion for agricultural management
LEACH-N	Hutson, *et al.*, 1991	Leaching estimates and chemistry model, N sub-model
NDSS	Rossiter, 1990	Nitrogen decision support system, N fertilizer calculation
NITROP	Osmond, 1991	Nitrogen fertilizer recommendation for maize in the tropics
NLEAP	Shaffer, *et al.*, 1991	Nitrate leaching and economic analysis package
NTRM	Shaffer, Larson, 1987	Nitrogen tillage and residue management
QUEFTS	Janssen, *et al.*, 1990	Quantitative evaluation of the fertility of tropical soils
PULSE	Bergstrom *et al.*, 1987	Simulation of runoff and nitrogen leaching from fields
SLIM	Addiscott, 1982	Nitrate movement in the field
SOILN	Johnsson, *et al.*, 1987	Simulating N dynamics and losses in layered soils
SUNDIAL	Smith, *et al.*, 1996	Turnover model, simulation of N dynamics in arable land
TORBERT	Torbert, *et al.* 1994	Simulation of soil-plant N interactions for educational purposes

modules that simulate various N cycle processes in soil-plant systems. SOILN model (Johnsson *et al.*, 1987), for example, was designed to simulate N dynamics and losses in layered soils. It consists of the main processes that determine the inputs, transformations, and outputs of nitrogen in arable soils. The components include fertilizer, manure, atmospheric deposition, mineralization, immobilization, leaching, denitrification, and harvest yield. So a good N model would be a very helpful tool in decision making for N management.

As discussed in the previous section, removing pollution completely from groundwater is almost impossible; cleaning may take years or decades and be extremely costly. The best way to control nitrate contamination may be to prevent it in the first place: where nitrogen fertilizers are applied. Therefore, proper nitrogen nutrient management is considered as a crucial part of the solution to nitrate pollution. As an important component of precision agriculture, precision nitrogen management has been proposed over the few past years (Robert *et al.*, 1996). Computer nitrogen modeling is an important part of precision nitrogen management. In this study, the knowledge "gaps" between the requirements of precision nitrogen management and existing nitrogen models were discussed first by evaluating existing models in Chapter 3. To fill the "gaps," a modeling method with artificial intelligence technologies, Management-Oriented Modeling (MOM), was developed in Chapter 5. MOM simulator, a dynamic N model was designed and tested as reported in Chapter 4. Finally MOM-guided within-season management was discussed with scenarios to illustrate the potential uses of MOM technology in precision nitrogen management in Chapter 6. Hopefully this study will contribute to the improvement of the environment quality and food production, as well as contribute to the rapid development of precision nitrogen management in precision agriculture, which is called the foundation for the next agricultural revolution (Robert, *et al.*, 1996).

Chapter 2

Materials and Methods

2-1. Criteria of Model Evaluation

Model evaluation in this study involved learning existing N modeling technologies and identifying the knowledge "gaps" needed to be filled. Potential evaluation criteria to evaluate models are numerous. For example, two lists of standards, mandatory and desirable criteria, were suggested by Meyer (1990) in Table 2-1.1 and Table 2-1.2.

Table 2-1.1. Mandatory user-interface standards of evaluating models †

1.	Introductory screen(s) displaying the information about authors.
2.	Introductory description for inputs.
3.	Introductory description for how to get "Help" and "Why" questions.
4.	Checking inputs to verify valid responses.
5.	At least some "Why" response available for all questions and "Help" for all but trivial queries.
6.	Some facility within the program to explain the logic pursued to reach the conclusion(s).
7.	Documentation for the program, running instructions, installation, technical support, and information on limitations of the system.
8.	Maximum delay of 5 seconds between a user response and a program response.

† Simplified from Meyer (1990).

Table 2-1.2. Desirable Standards of evaluating models ‡

1.	Ability to enter all responses in upper or lower case.
2.	All inputs are made via a routine that checks for Help and Why.
3.	Reminds user to get Help or ask Why at each response if needed.
4.	Clears the screen before each question is displayed.
5.	Actions required of user are highlighted to attract user's attention.
6.	User can save current run to a disk file.
7.	User can back up to the previous question if desired.
8.	Provide an operating-system shell.
9.	At each question, tell the user where he/she is in the run.
10.	The program can be rerun without returning to the operating-system.
11.	Help screens can be selected to explain the equations and logic used.
12.	Explanations are displayed in common English rather than using an internal rule language.
13.	A two-level Why/Help system for novice users to get detailed answers.
14.	The ability to edit responses from previous run, and rerun without re-entering all data.

‡ Simplified from Meyer (1990).

Statistical criteria and graphical displays have been also used to evaluate models (Loague and Green, 1991). These criteria are useful to assess N models. Additional criteria described below were designed as an outline to guide the evaluation.

2-1.1. Purposes

- What are the **objectives** of the system?
- What **problems** can be solved? What **benefits** might be obtained from use of the system?
- What **functions** does the system perform? (interpretation, prescription; diagnosis, repair, prediction; design, configuration, planning; monitoring, control; instruction; or others)

- Who are the potential **users**? (farmers, land owners, government planners, agencies, extension specialists, research institutes, universities, the public, and others)
- Can the system address multiple **user skill** levels?

2-1.2. Inputs and Outputs

- Are there **scenarios** or **examples** to guide data entry?
- What is the **minimum data set** (Nix, 1984)?
- Is the information required difficult or expensive to acquire?
- How does the system handle **default situations**? (default system's parameters, user's databases, other methods)
- What are major **outputs** (results such as predictions, conclusions, or recommendations) produced by the system?
- What methods are used to **manage user data**? (specific databases, spreadsheets, keyboard entered only, others)

2-1.3. Suitability

- How does the system **adapt** to various agricultural regions? (user-oriented databases, system parameters, other approaches)
- Is there documented **validation** in different regions?

2-1.4. Software

- What development **strategies** (knowledge representation methods) were used? (statistical, mechanistic, simulation, symbolic reasoning, or others)

- What development **tools** were used? (e.g., C++, Pascal, Prolog, Lisp, or expert system shells)
- Is the system **interface** attractive, friendly, and helpful?
- Are there **structure diagrams** that describe the system to users?
- Are the procedures "**transparent**" (open to view if desired) to the users?
- How does the system deal with **errors** and online **help**?
- Does the system offer **user-guidance**? (manual, readme files, examples, demonstrations, tutorial programs, installation information, troubleshooting, feedback)
- Is the system easy to **upgrade**? Is its knowledge **renewable**?

2-1.5. Conclusion

- What are the major **strengths** and **limitations** of the system?

Above criteria will be used to evaluate nine existing nitrogen models.

2-2. Tools of Model Development

In order to reach the objectives of this study, discussed in section 4-1.1, the development tool must meet several programming requirements. First, the development tool must be able to compile source code to native machine code for a high-speed simulator. The simulator may be required to complete hundreds of simulations of the N cycle in soil-plant systems during a whole cropping season in acceptable simulation time. For example, the simulation of 100 cropping seasons should be finished in 5-10 minutes on current personal computers. Second, the tool should have database development capability and it should easily access commercial databases. The proposed models must have a common input/output connection with popular commercial software to facilitate use by multiple users for multiple purposes. Third, the tool should be a visual programming for Windows applications with Integrated Development Environment (IDE). This will help focus the modelers' creativity on the knowledge construction of models, rather than simply producing Windows interfaces of the models. After comparing many computer programming languages and shells, Borland Delphi [1] nearly matches the requirements and was chosen as the main development tool for the proposed N models. Delphi is a Rapid Application Development (RAD) tool for Microsoft Windows with Object Pascal. It encapsulates database components that can assess Paradox, dBASE, and ODBC tables. Delphi also has a visual, object-oriented, and component-based Integrated Development Environment.

2-3. Methods of Model Tests

Two procedures, verification and validation, are often used to test biological models. Verification comprises the comparison of the structure and general behavior of a model with the real system and ensuring that the model operates on the data in the intended way (Jeffers, 1978; Carter, 1986). A trial-and-error method of verification changes parameter values to improve the fit of the model to observations. In verifying the model developed in this study, the trial-and-error method was employed to calibrate

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[1] Use of specific software does not imply or suggest endorsement by author, committee, or University of Hawaii. Other software may meet the model requirements but was not evaluated.

some parameters that were not available from datasets, literature, or fields and experiments. Validation refers to comparison of the model output with observations not used to develop the model (Jeffers, 1978; Carter, 1986). The following methods are usually used to validate agricultural models.

(1) Graphically represent the predicted and observed results with or without associated confidence limits (Grant, 1989, Ingram and McCloud, 1984; Jones *et al.*, 1980; Jones *et al.*, 1991; Loague and Green, 1991; Ling, 1996).

(2) Simply compare the predicted and observed data using 1:1 line graphs without testing hypotheses (Jones *et al.*, 1980; Jones and Kiniry, 1986; Albers and Ward, 1991; Godwin and Jones, 1991).

(3) Compare the closeness of the predicted and observed data by agreement index (Albers and Ward, 1991).

$$AgreementIndex = 1 - \frac{|PredictedValue - ObservedValue|}{ObservedValue}$$

(4) Use mean squared error, root mean square error, standard deviation, coefficient of determination between the observed and predicted values (Wallach and Goffinet, 1989; Loague and Green, 1991).

(5) Use linear regression analysis of observations against the predicted to test the hypothesis that the regression line should have a slope not significantly different from unity and an intercept not significantly different from the origin (Draper and Smith, 1966; Dent and Blackie, 1979; Zhang, 1992).

Carter (1986) suggested two important criteria for biological simulation models: (1) is the general shape of the curve correct? (2) is the quantitative agreement reasonable? Graphical representation of model predictions and observations was used to evaluate the models developed in this study with all datasets. Quantitative evaluating a biological model with statistical tests has been questioned by many investigators. For example, root mean square error was criticized as a poor indicator of the performance of models, which gives no indication of bias (Mitchell and Sheehy, 1997). Regression as a quantitative method of empirical validation, another example, has been questioned as a misapplication (Harrison, 1990; Mitchell and Sheehy, 1997). They argued that this kind of regression application was (1) not satisfying the regression assumptions, (2) ambiguous results of null hypothesis tests, and (3) fitted line being irrelevant to model performance. However, regression was promoted as a quantitative method to statistically validate models by other investigators (Reckhow *et al.*, 1990; Flavelle, 1992; Mayer *et al.*, 1994). Little and Hills (1978) suggested that linear regression can be employed to analyze two types of data: (1) The data that conform to *model I* in which the X values are fixed and usually refers to the independent variable. (2) The data that conform to *model II* in which X values are random or subject to error. An example of regression of data that conform to *model II* is dealing with *bivariate normal distribution*. Neither variable can be designated as dependent on the other in this case. A reasonable degree of closeness of the two variables is primarily interested, not estimating the value of one variable from the other (Little and Hills, 1978). Linear regression with pairs of model predicted and observed data may be a *model II* regression problem.

Because the statistical validation of models has been open to question and the primary purpose of this study is not to evaluate validation methods, a simple 1:1 line scatter graph was used to evaluate model accuracy. The term of *model accuracy* in this study refers to the degree of agreement or closeness between the model predicted results and observed data, not to the degree of closeness between the model predictions and the **true** values in the real-world.

2-4. Datasets of Model Tests

In this study, dynamic N data refer to N status of a soil-plant system measured at several intervals during the experimental period in addition to the initial measurement. Other measured data included daily or weekly rainfall, ET, or temperature. A total of eleven dynamic N datasets were collected from Hawaii and Brazil. The datasets represent a range of conditions described by three crops at five locations and a laboratory experiment.

2-4.1. Maize, Legume Green Manure Experiment, Brazil

Two datasets that were used for testing the CERES-Maize model, maize (*Zea mays L.*) cropped with a legume green manure and control, were provided by Dr. Bowen (IFDC, P.O. Box 2040, Muscle Shoals, AL 35662). The data came from the three irrigated dry season experiments and one rainfed wet season experiment that were conducted at the Cerrado (Savanna) Agricultural Research Center (CPAC-EMBRAPA; 15°35' S, 47°42' W) near Brasilia, Brazil from 1984 through 1987. The soil of the experiments was classified as *clayey, oxidic, isothermic Anionic Acrustox* (Bowen *et al.*, 1988). The data used for our simulation came from the experiment during the 1984-1985 wet season. In the experiment, a commercial maize hybrid (Cargill 111) was planted on Dec. 26, 1984 and harvested May 24, 1985 during the wet season (rainfed). An amount of 5590 kg ha^{-1} of green manure with 3.33 % N content, a legume species (*Mucuna aterrima* (Piper & Tracy) Merr.), was incorporated three days before planting as green manure (GM) fertilizer treatment. No surface residue was incorporated as the control treatment. Both the GM treatment and the control received 10 kg N ha^{-1} urea fertilizer three days before planting. The experiment design was a randomized complete block with four replicates. The soil profile was sampled in 15 cm increments to a depth of 120 cm. Inorganic soil nitrogen was analyzed using the steam distillation method (Keeney and Nelson, 1982).

2-4.2. Maize, N Fertilizer Experiment, Hawaii

A field experiment of maize with N fertilizer was conducted by the Benchmark Soil Project (Benchmark Soil Project Staff, 1982) in Waipio, Oahu, Hawaii (approximately 21°25' N, 158° W), November 1983 to April 1984. The soil is an Oxisol *(Wahiawa series)* with moderately rapid permeability and slow runoff. A randomized complete block design was used for the experiment with three N levels (0, 51, 201 kg N ha^{-1}), two varieties of maize ('X304C', Pioneer Hi-Bred International; 'H610', Ant 2D x B14A), and three replicates. The experiment was originally designed to study effects of variety and N rates on maize growth and yield (Singh, 1985). The maize was planted on November 30, 1983 and harvested on April 15, 1984. Drip irrigation was applied when tensiometer readings were less than 0.2 MPa. Dr. Gordon

Tsuji (Benchmark Soil Project, CTAHR, University of Hawaii) provided two datasets from the experiment for this study. The datasets were from maize variety 'X304C' with urea treatments of 51 and 201 kg N ha^{-1}, which were split in three applications.

2-4.3. Maize, Field Sampling, Hawaii

Datasets of nitrate content in soil profiles from maize fields, sugarcane fields (See section 2-4.4) and pineapple fields (See section 2-4.5) in Kunia and Wahiawa, Oahu, were provided by Dr. El-Kadi (Department of Geology and Geophysics, University of Hawaii at Manoa, 1996) and Dr. Ling (Department of Geology and Geophysics, University of Hawaii at Manoa, 1996). Total of 5,048 soil samples were collected for the project "Nutrient Use Assessment in the Kunia Watershed" from 1993 to 1994 (El-Kadi, 1996). The field information of cropping, irrigation and fertilization, soil sampling and analysis procedures were described in detail in Ling's dissertation (1996). A brief description of the datasets follows.

The sampled maize fields, ICI Seeds Company, are located in Kunia, a central Oahu watershed. The soil is an association of an Inceptisol (*Kunia* series) with an Oxisol (*Wahiawa series*). The sampled fields are located within the mapunit KyA (Kunia silty clay) but only about 100 m to the very highly weathered soil in mapunit WaA (Wahiawa silty clay). A total of 1452 soil samples were collected with 10 cm bucket augers from 12 holes to a depth 150 cm (11 soil layers) over about one hectare for two cropping seasons. Nitrate was analyzed for all soil samples while ammonium was determined only in selected samples. Winter maize was planted on Nov. 12, 1993, four days after the first soil sampling. Fertilizer UAN-32 (a mixture of urea, ammonium and nitrate) was applied for four times during the cropping. The crop was irrigated. Summer maize was planted on May 26 and harvested on September 1, 1994. Soils were sampled beginning on May 23, 1994. Fertilizer UAN-32 was split into three applications on June 10, June 23, and July 7, 1994.

2-4.4. Sugarcane, Field Sampling, Hawaii

Soil samples were collected from a sugarcane field of Waialua Sugar Company, near the UH Poamoho Experiment Station, Oahu, Hawaii. The soil is an Oxisol (*Wahiawa series*). Total of 559 soil samples were collected from 12 holes to a depth 150 cm (11 soil layers) over four hectare area to analyze for nitrate content. Sugarcane was planted on June 16, 1994. The crop was irrigated and a liquid urea fertilizer, Urea-46, was applied during the crop.

2-4.5. Pineapple, Field Sampling, Hawaii

The pineapple dataset consists of soil nitrate analysis data for a total of 2640 soil samples collected from 24 holes with 11 soil layers to a depth 150 cm over three hectare area during first 400 days of cropping. The sampled field, on Del Monte Fresh Produce Inc. land, is located in Kunia, Oahu, Hawaii, where soil is an Oxisol (*Wahiawa series*). Pineapple was planted on September 30. During sampling period, fertilizer UAN-32 was applied using truck-mounted sprayers on the 64, 76, 83, 90, 98, 119, 154, 161, 180, 191, 196, 218, 226, 230, 237, 249, 259, 266, 278, 295, 314, 326, 334, 364 days of after planting.

2-4.6. Nitrate Leaching, Column Experiment, Laboratory

Jonathan L. Deenik (1997) provided a nitrate leaching dataset from a soil column experiment in the laboratory. The soil column experiment was originally conducted to measure the effect of surface applied lime and gypsum on nitrate mobility in subsoil. An Oxisol (*Wahiawa* series) and an Ultisol (*Leilehua* series) were used in the experiment, collected at two depths (the surface layer, 0-15 cm, and the subsoil, 80-100 cm) from sugarcane fields in the Waialua area of Oahu, Hawaii. The soils were air-dried, sieved and packed into PVC columns to form soil columns with the diameter of 5.6 cm and height of 51 cm (15 cm of surface soil, 36 cm of subsoil), achieving a bulk density of 1.0 g cm^{-3}. Before packing, the surface soils were mixed with 0.355 g KNO_3 (equivalent of 200 kg N ha^{-1}) for each column, 0.36 g of $Ca(OH)_2$ (equivalent of 4 ton ha^{-1}) and 0.68 g of $CaSO_4$ (equivalent of 3 ton ha^{-1}) for corresponding treatments. Forty ml of deionized water was added to the columns in 10 ml increments at a set time once daily to simulate a 16.2 mm daily rainfall over the leaching period. Leachate was collected and analyzed for nitrate every two days. The experiment was executed in three replicates. The *Leilehua* columns and the gypsum treatment of the *Wahiawa* soil columns were dismantled after 6 weeks while the control and lime columns continued for additional 2 weeks.

2-5. Soil Sample Analysis

In addition to collected datasets, soil ammonium, nitrate and nitrate adsorption coefficients in Hawaii soils were determined by the procedures described below.

2-5.1. Soil ammonium and nitrate

Soil samples (of Hawaii in sections 2-4.3, 2-4.4, 2-4.5) were stored in the freezer room until analysis. 7.000 g of soil samples at field moisture were weighed into 100 ml plastic cups to which 50 ml of 2*M* KCl solution was added. The cups were covered and agitated on an automated shaker for two hours. Then the supernatant liquid in the cups was filtered through a medium filter paper (pre-treated by deionized water to remove ammonium and nitrate). The extracted liquid was analyzed for ammonium colorimetrically (Willis and Gentry, 1988) and for nitrate by the colorimetric cadmium reduction method (Maynard and Kalra, 1993).

2-5.2. Nitrate adsorption coefficients

Duplicate 7.000 g soil samples at field moisture and 25.00 ml of 3.000 *mM* nitrate were placed in pre-weighed 40 ml plastic centrifuge tubes (soil:water 1:5). The tubes were agitated for two hours (Cahn, 1992) to reach equilibrium nitrate adsorption, then centrifuged at 5000 RPM for 10 minutes. The supernatant was decanted and weighed, then filtered through a medium filter paper. The supernatant was analyzed for nitrate with the colorimetric cadmium reduction method (Maynard and Kalra, 1993). The tubes with soil and trapped soil solution were weighed for calculation of total remaining nitrate. One of the duplicate samples was extracted with 25.00 ml of 2 *M* KCl and analyzed for total nitrate remaining in the tube. This total amount includes soil initial nitrate. To another sample, 25.00 ml of 5 *mM* KCl solution was added (the ionic strength is close to the field level of tropical soils). The tube was agitated for two hours and centrifuged at 5000 RPM for 10 minutes. The supernatant was decanted and weighed, then filtered through a medium filter paper in preparing nitrate measurement with the colorimetric cadmium reduction method (Maynard and Kalra, 1993). The tube plus soil and trapped solution were weighed for calculation of current nitrate remaining in the tube. Then 25.00 ml of 5 mM KCl solution was added to the tube again and above steps were repeated 5-6 times until nitrate concentration of the supernatant was less than 0.5 mg L^{-1}. The remaining soil sample was extracted with 25.00 ml of 2 *M* KCl and analyzed for remaining nitrate in the tube.

Adsorbed nitrate in each of the displacement steps was calculated as follows:

In the **first** displacement step, Apply V_{ad} ml of 3.000 *mM* nitrate to the tube. The total nitrate (μg) in the tube is

$$T_1 = C_{ad} \cdot V_{ad} + T_{soil}$$

$$T_1 = Supernatant + Remains = C_1 \cdot V_1 + (C_1 \cdot V_{tp1} + T_{s1})$$

where,

C_{ad} = Concentration of nitrate standard solution (known)

V_{ad} = Volume of nitrate standard solution (known)

C_1 = Nitrate concentration of supernatant in first displacement (**measured**)

V_1 = Volume of supernatant in first displacement (measured or calculated)

V_{tp1} = Volume of trapped solution in first displacement (calculated)

T_{soil} = Total initial nitrate content in the soil (concept only)

T_1 = Total nitrate in the tube in first displacement (calculated)

T_{s1} = Total adsorbed nitrate in the soil in first displacement (calculated).

Because the bulk density of the 3 *mM* nitrate solution ≈ 5 mM KCl solution ≈ pure water, 1 ml volume of the solutions ≈ 1 g is acceptable in the experiment. Therefore, the **weight relationship** of centrifuge tubes, soil samples, and solutions is

$$Total = Solution(supernatant) + Tube + \underline{Solution(trapped) + Soil(oven\text{-}dry)}$$

$$= Solution(supernatant) + Tube + \underline{Remains}$$

So

$$V_1 = Total - (Tube + Remains)$$

$$V_{tp1} = Remains - Soil(oven\text{-}dry)$$

In the **second** displacement,

$$T_2 = C_1 \cdot V_{tp1} + T_{s1}$$

$$T_2 = C_2 \cdot V_2 + (C_2 \cdot V_{tp2} + T_{s2}) = C_2 \cdot V_2 + T_3$$

where,

C_2 = Nitrate concentration of supernatant in second displacement

V_2 = Volume of supernatant in second displacement

V_{tp2} = Volume of trapped solution in second displacement

T_2 = Total nitrate in the tube in second displacement

T_3 = Total nitrate in the tube in third displacement

T_{s2} = Total adsorbed nitrate in the soil in second displacement.

In the **third** displacement,

$$T_3 = C_2 \cdot V_{tp2} + T_{s2}$$

$$T_3 = C_3 \cdot V_3 + (C_3 \cdot V_{tp3} + Ts3) = C_3 \cdot V_3 + T_4$$

In the **nth** displacement,

$$T_n = C_{n-1} \cdot Vtp_{n-1} + Ts_{n-1}$$

$$T_n = C_n \cdot V_n + (C_n \cdot Vtp_n + Ts_n) = C_n \cdot V_n + T_{n+1}$$

Suppose displacement steps end at 5th displacement,

$$T_5 = C_4 \cdot V_{tp4} + Ts4$$

$$T_5 = C_5 \cdot V_5 + (C_5 \cdot V_{tp5} + T_{s5}) = C_5 \cdot V_5 + T_6$$

where T_6 = Total remaining nitrate, measured by 2M KCl extraction. Therefore,

$$T_{s5} = T_6 - C_5 \cdot V_{tp5}$$

Generally, for nth displacement,

$$Ts_n = T_{n+1} - C_n \cdot Vtp_n$$

where, Ts_n / soil weight refers to **Adsorbed Concentration**. C_n is **Solution Concentration** (measured supernatant). An isotherm of nitrate adsorption against the equilibrium solution is then plotted. A Freundlich equation is usually used to express the adsorption.

$$X = a \cdot C^b, \text{ or}$$

$$Log\,X = Log\,a + b\,Log\,C$$

where, $X = N_s$ (mg nitrate kg $^{-1}$ dry soil) is the amount of adsorbed nitrate. $C = N_t$ (mg nitrate L $^{-1}$ solution) refers to the amount of nitrate remaining in soil solution. The equation parameters a and b are nitrate adsorption coefficients. For low nitrate concentrations in field conditions, parameter a could be simply used as adsorption coefficient:

$$K_{NO3^-} = a = X / C$$

Moreover, nitrate adsorption coefficients (a and b) can be used to estimate the amounts of nitrate **adsorbed** and nitrate **remaining in solution**. Assume

Total (nitrate) = Adsorbed + Remaining in Solution

T = total nitrate in soils (mg nitrate kg $^{-1}$ dry soil, usually estimated with a 2 M KCl extraction).

X = nitrate adsorbed on the soil solid phase at field moisture (mg nitrate kg $^{-1}$ dry soil).

W = field moisture determined by weight percentage (g solution/g dry soil).

C = nitrate remaining in soil solution (mg nitrate L $^{-1}$ solution, or mg nitrate kg $^{-1}$ solution, assume the bulk density of the soil solution ≈ 1).

Then,

$$T = X + W \cdot C \quad \Rightarrow \quad T = a \cdot C^{b} + W \cdot C$$

Therefore,

a) if T (2 M KCl extraction of soils) is measured, C can be calculated by $T = aC^b + W \cdot C$, and then X can be calculated.

b) if C (soil solution) is measured, T can be calculated by $T = aC^b + W \cdot C$, and then X can be calculated.

Chapter 3

Evaluation of Existing Nitrogen Models

Many N models have been developed since the 1980s (See section 1-2). In order to examine whether these models provide output to satisfy our proposed goals of N management, nine computer programs of the N model were collected to evaluate under the guidance of the criteria described in section 2-1.

3-1. NDSS: Nitrogen Decision Support System

3-1.1. System Purposes

NDSS was designed to help users estimate crop N fertilizer requirements. Its recommendations are helpful in reducing environmental contamination by appropriately applying nitrogen fertilizers, though NDSS was not primarily designed as a dynamic model to assess nitrogen leaching. With local database support, farmers and extension technicians should be able to use NDSS for the N fertilizer management. To estimate the amount of nitrogen fertilizer needed, NDSS uses an adaptation of the Stanford Equation (Stanford, 1973; Rossiter, 1990):

$$N_{required} = \frac{N_{crop} - N_{soil} - N_{rotation} + N_{loss} + N_{rootzone}}{E_{fertilizer}} - N_{manure} \qquad [3\text{-}1.1]$$

3-1.2. System Inputs & Outputs

NDSS associates equation [3-1.1] with four kinds of databases as inputs:

1. Crop databases that contain the N contents of crops.
2. Soil databases that describe N supplied from soils with the soil characteristics (e.g., soil name, drainage, tillage depth) and corresponding N utilization efficiencies.
3. Fertilizer databases that describe N contents in different fertilizers with their formulas.
4. Application records in which user's site data are stored. Besides soil and fertilizer information, data regarding the rotation of crops, animal and green manures are saved in each record.

NDSS provides several default data sets with the package. The default value of N fertilizer efficiency was 0.65 ($E_{fertilizer}$ in equation [3-1.1]). However, users can establish user databases for crops, soils, fertilizers and application sets. All N components in the equation [3-1.1] are displayed during NDSS calculation. NDSS output includes the recommended amount of N fertilizer plus some brief comments.

3-1.3. System Suitability for Various Regions

NDSS should be adaptable to specific sites using local soil and crop databases without requirements of weather data. However, recommended fertilizer may vary with the value of the N fertilizer efficiency in the Stanford Equation, which varies with soils, crops, climates and management practices (Malzer and Graff, 1984, 1985, Bock and Hergert, 1991). A large variation would result between actual and predicted N requirements if estimates of fertilizer efficiency do not fit local conditions.

3-1.4. Software & Hardware Environment

NDSS was developed using Microsoft Foxpro 2.0 [1]. Besides the default databases provided by NDSS, users can store and retrieve their local data in the user's databases. NDSS's procedures were explained by online help (F1 or F2 function keys), which can 'pop-up' anywhere in the program. F1 gives information on the program and what to do next. F2 explains how a quantity is calculated. NDSS allows users to change default values, databases and settings, including some general settings such as 'colors', 'units' and the 'ID at startup'. A DEMO dataset was provided to guide the usage of the software.

3-1.5. Conclusion

NDSS is very useful in estimating N fertilizer requirements without the dynamic N behavior. The advantage of the model is its minimal data requirements supported by soil and crop databases. If the fertilizer utilization efficiency were linked to soil, crop,

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[1] The mention of specific software does not imply or suggest endorsement by author, committee, or University of Hawaii. The discussion would apply to the software mentioned in following chapters.

weather, and management factors, the model prediction would fit various situations better.

3-2. QUEFTS: QUantitative Evaluation of the Fertility of Tropical Soils

3-2.1. System Purposes

QUEFTS was developed to evaluate NPK fertilization needs (Janssen *et al.*, 1990). It estimates the potential NPK supply from soils, the "actual" NPK uptake by crops, and yields. The system is useful for farmers to balance NPK fertilization and economic optimization. However, the environmental impact of fertilization was not evaluated by QUEFTS. Using a mechanistic approach, QUEFTS takes four steps from soil properties to crop yields: soil parameters → potential nutrient supply → actual nutrient uptake → possible yield ranges → final yield estimation. Relations between the steps are determined by a series of fertilizer trials on local soil and climate conditions. For example, the fertilizer recovery fraction must be calibrated by users for their crops, soils and climate.

3-2.2. System Inputs & Outputs

QUEFTS requires soil data of pH, organic C and N, Olsen P and exchangeable K. The output is a list of yields, value of yields, fertilizer costs and net return to the fertilizer. Total outputs correspond to a maximum of 70 combinations of fertilizer rates. Farmers can choose the best rate to meet their desired yields or net returns. A rate may be "nutritional optimum" according to optimum yields, but may not be the economic optimum. The authors found a maximum "total yield-producing uptake efficiency" at 0.96 under a potential supply ratio of N:P:K = 7.8:1.0:5.8. QUEFTS weighs financial optimization more than nutritional optimization and provides a financial optimization procedure.

3-2.3. System Suitability for Various Regions

QUEFTS was developed and tested at the Agricultural University of Wageningen, Netherlands. It looks as a promising tool for evaluating native fertility of tropical soils. QUEFTS was distributed with default soil parameters from Kenya and Surinam, where soils are deep, well drained and with properties listed below.

Soil Properties of the Default Parameters	
pH (H_2O)	4.5 -- 7.0
Organic Carbon	< 70 g C kg^{-1}
P-Olsen	< 30 mg P kg^{-1}
Exchangeable K	< 30 mg K kg^{-1}

If users' soils and climate conditions are significantly different from the default sites, QUEFTS's parameters must be reinitialized by users. Initialization requires users to calibrate equation coefficients with local fertilizer experiments. So, the system would work for various regions if the parameters can be estimated from local experiments.

3-2.4. Software & Hardware Environment

QUEFTS is a combination of statistical and mechanistic models developed using Turbo Pascal 5.0. All data are entered and edited through the keyboard, then saved to files. Online help guides users step by step and controls data entries within reasonable ranges. As a simple system, QUEFTS runs either on a floppy or a hard disk with a little working memory. The manual clearly documents the equations and parameters in the model.

3-2.5. Conclusion

In estimating yields, QUEFTS assumes that no serious growth limitations exist other than soil fertility. If the coefficients are calibrated to local conditions, QUEFTS is a useful tool to optimize the combinations of NPK fertilizers and net return on static basis without evaluating impacts on the environment.

3-3. NITROP: Nitrogen Fertilizer Recommendation for Maize Produced in the Tropics

3-3.1. System Purposes

NITROP (Osmond, 1991) is an expert system designed to determine nitrogen fertilizer requirements for maize in tropics. It consists of three N models: Stanford Equation, Transfer Coefficient Method, and N Mass Balance Equation. Users can choose one or more of the models to predict N fertilizer for the target yields. The Stanford equation (Stanford, 1973) was expressed in NITROP as

$$N_{fert} = (N_{crop} - N_{soil}) / E_{fert} \qquad [3\text{-}3.1]$$

where N_{fert} is required N fertilizer. N_{crop} refers to N absorbed by the crop and N_{soil} refers to soil supplied N. E_{fert} is the efficiency of fertilizer utilization. The second model, the DeWit/Wolf transfer coefficient model (Wolf, 1989), expresses N_{soil} as a sum of N transferred to the crop from the soil. The recommended fertilizer is

$$N_{fert} = \frac{N_{crop} - \sum E_i \cdot N_{input}}{E_{fert}} \qquad [3\text{-}3.2]$$

The third model, a nitrogen mass balance equation, calculates a nitrogen fertilizer requirement from the difference between N out of the soil system and N into the soil system:

$$N_{fert} = \frac{\sum N_{losses} - \sum N_{gains}}{E_{fert}} \qquad [3\text{-}3.3]$$

Three models have stated that the amount of N required is the difference between N removed by crops and N supplied from soils. Different equation coefficients sometimes resulted in different predictions (Osmond, 1991). This is not surprising because the coefficients are actually functions of many soil-plant processes, and this are not constants. In many cases in which no appropriate local coefficients are available, models have to use constants as defaults even though these constants may not represent state-of-the-art conditions for the sites.

3-3.2. System Inputs & Outputs

NITROP has eight subroutines of inputs: 1) total aboveground N content in dry matter for the fertilized crop; 2) total aboveground N content in dry matter for the unfertilized crop; 3) the N fertilizer efficiency; 4) the N in rainfall; 5) mineralized N; 6) stover N; 7) preceding crops; and 8) leached N. All data are input from the keyboard without using databases. Default values are available in NITROP except soil organic matter and crop yield goal. Output was the N requirement by proposed maize, calculated by the Stanford Equation, the Transfer coefficient Method, or N Mass Balance Equation.

3-3.3. System Suitability for Various Regions

NITROP was evaluated using seven datasets, three from South America and four from Africa. The Stanford Model gave good predictions at many locations (Osmond, 1991). The key coefficient in the three models was the N fertilizer efficiency. It was estimated from soil texture, rainfall, fertilizer types, pH, natural vegetation and cropping history in NITROP. This approach makes NITROP suitable for various areas. Like NDSS, calibrations of the fertilizer efficiency from local data are necessary for an accurate prediction.

3-3.4. Software & Hardware Environment

NITROP was developed using VP-Expert (version 2.1). VP-Expert is a rule-based expert system shell. The reasoning strategy of NITROP is backward chaining, which means the system evaluates potential conclusions by determining the necessary supporting data for each rule and calculation. Users can easily learn and use this system with the VP-Expert interface. Like most expert systems that take advantage of the development shell, NITROP answers users' questions of "How" for variable values and "Why" for its reasoning and computation. Online help and error controls in NITROP are provided by the VP-Expert shell. The system description was available in the author's dissertation.

3-3.5. Conclusion

NITROP was designed as the same tool as NDSS to estimate N fertilizer requirements. NITROP uses the expert system shell. The system limitations come from its assumptions: 1) the only limiting soil nutrient is nitrogen; 2) good agronomic practices will be followed; 3) normal climatic conditions will prevail, and 4) reliable estimates of fertilizer efficiency are available.

3-4. NLEAP: Nitrate Leaching and Economic Analysis Package

3-4.1. System Purposes

NLEAP was designed to rapidly estimate nitrate-N leaching potential by examining nitrate loss processes through the combination of chemical, physical and biological sub-processes (Shaffer, *et al.*, 1991). Potential users may be extension personnel and action agencies such as Natural Resources Conservation Service (NRCS) and Environmental Protection Agency (EPA). The model evaluates nitrate impact on the environment and economic crop production. Nitrate leaching risk was evaluated by indices related to precipitation, soil texture and temperature. NLEAP provides three screening analyses: 1) an annual analysis for initial estimates of potential nitrate leaching, 2) a monthly analysis, and 3) an event-by-event analysis for more detailed N budget information.

3-4.2. System Inputs & Outputs

NLEAP stores site specific soil and climate data in its internal databases. Major data required include: 1) inputs of N into the root zone such as mineralized N, crop residue N, fertilizer N, and precipitation N, 2) removal of N from soils such as crop harvest, runoff, and gaseous loss, 3) soil properties such as bulk density, pH, CEC, soil texture, and soil water content, 4) crop management data, 5) irrigation data, 6) simple aquifer data, 7) climate data such as precipitation and temperature. Outputs consist of indices and a text report. The indices provide a qualitative assessment of nitrate leaching in movement risk, annual leaching risk, and aquifer risk. The report provides a discussion of results and recommendations for management. These results are helpful in understanding and reducing nitrate leaching of the sites.

3-4.3. System Suitability for Various Regions

NLEAP was validated with lysimeter and groundwater data obtained from Ohio, Minnesota, Nebraska, Iowa, and Michigan. NLEAP predictions were compared with 5-yr observed values for nitrate leached from USDA-ARS lysimeter Y103 B located at Coshocton, OH. The results indicated that 91% of the variability in leaching volume and 86% of the mass of nitrate leached were predicted by NLEAP. The authors restricted using NLEAP to assess potential nitrate leaching into sources of domestic water supply.

3-4.4. Software & Hardware Environment

NLEAP's interface was written in Microsoft C (version 6.0) and the computations were written in Microsoft FORTRAN 77 (version 5.0). Information of installation, hardware and software requirements, and troubleshooting was documented in two readme files with the software package. The model description was published by Shaffer *et al.* (1991).

3-4.5. Conclusion

NLEAP is a useful tool to qualitatively assess annual and monthly nitrate leaching risks or the risk associated with water events. The limited dynamic module of event-by-event analysis (using daily rainfall and irrigation data) improved the assessment of nitrate leaching. NLEAP may be a useful model for the assessment of watershed level if integrated with GIS, standard databases and graphic user interfaces.

3-5. AGNPS: Nonpoint-Source Pollution Model for Evaluating Agricultural Watersheds

3-5.1. System Purposes

AGNPS was developed to estimate runoff water quality from agricultural watersheds (Yong, *et al.*, 1989). The estimates can be used to compare the performance of selected watersheds experiencing similar runoff events. The potential users are professionals with knowledge of hydrology, soil science, agronomy, and climatology. Basic model components include hydrology, erosion, sediment and chemical transport. In addition, the model considers point sources of sediment from gullies and inputs of water, sediment, nutrients, chemical oxygen demand (COD) from animal feedlots, and springs, etc. AGNPS uses the measure of COD as an indicator of pollution.

3-5.2. System Inputs & Outputs

AGNPS operates on a cell basis. Cells of uniform square areas subdivide the watersheds, allowing analysis at any point within the watershed. Watershed characteristics and inputs are expressed at the cell level. Potential contaminants are routed through the watershed cell by cell. Therefore, flow at any point between cells can be examined. Each cell was described by 19 variables such as land slope, nutrient, chemical oxygen demand (COD), soil, fertilization, and gully and others. Consequently, a large amount of data was required to run AGNPS. For instance, in 12,920 acres of Eagle Lake watershed area, an example from the package, there were 6,137 data within 40 cells. The database of AGNPS was specified by the model. Users must enter all data in the internal spreadsheets by keyboard. Major outputs consist of runoff, sediments, and chemicals including nitrogen, phosphorus and COD at the watershed outlet or at a cell. Besides tabular output, simple maps based on cells of watersheds can be viewed on the screen.

3-5.3. System Suitability for Various Regions

AGNPS was validated for runoff with data from 20 different watersheds in the north central US. Parts of the model have been tested for sediment yield estimates with data from two experimental watersheds in Iowa and Nebraska. The chemical components of AGNPS have undergone basic testing since 1989.

3-5.4. Software & Hardware Environment

AGNPS was originally developed with the FORTRAN 77 and the latest version (ver. 4.0) was written in C. It has a full-screen data entry editor and help screen. PC version can control a maximum of 1,900 cells. Online help gives users assistance to operate the system. Users can learn the model through several examples provided with the package or the User's Guide.

3-5.5. Conclusion

AGNPS is a useful event-based assessment tool with simple maps that estimates surface water pollution by runoff, sediment, and nutrient (N and P) transports from agricultural watersheds. A major task is obtaining and entering extensive data from the watershed to fill the thousands of AGNPS cells for diagnosis or prescription in watershed management.

3-6. CERES-Maize: Simulation Model of Maize Growth and Development

3-6.1. System Purposes

CERES (Crop Environment Resource Synthesis) Maize (*Zea mays. L.*) model was developed to simulate maize growth, development and yield (Ritchie *et al.*, 1986). It consists of two versions: standard and nitrogen versions. The standard version simulates the effects of cultivar, planting density, soil water, and daily weather on maize growth. The nitrogen version, called CERESN, includes components of standard version plus soil-plant nitrogen dynamics for the crop. CERES-Maize was designed for agronomists, teachers, extension service, cropping consultants, farmers, and others who work with the crop.

3-6.2. System Inputs & Outputs

- **Inputs**

Two types of input data, the parameters and daily weather data, were used in CERES-Maize. Parameter inputs are used to assign values to the variables that control the execution and initialize pools. They include:

1) Switches that control the model execution.
2) Soil layer data: the thickness of the layer, the lower limit of plant-extractable water, the drained upper limit, the water content at saturation, a weighting factor for rooting, initial soil moisture, pH, organic carbon, ammonium, and nitrate.
3) Management input of irrigation amount and frequency, fertilizer application rates.
4) Genetic coefficients for the cultivar.
5) Measured data such as silking dates and grain yield to be used as comparisons with simulation results.

Daily weather data include day of the year, solar radiation, maximum and minimum air temperature, and precipitation for each day simulated.

- **Outputs**

The simulation outputs three files including following data:

1) Crop growth, development, yield, and soil nitrogen and moisture.
2) Daily plant growth information including dates, number of leaves, leaf area, weight of root, straw, grain and leaf, root depth and root length density.

3) Daily water balance results including dates, plant transpiration, evapotranspiration, solar radiation, temperature, precipitation, and volumetric soil water content in the surface five soil layers.

The nitrogen version outputs additional information of N in grain, leaf, stem, shell, root, and soils. Soil N contains nitrate and ammonium in soil layers, organic N, and leachate N.

3-6.3. System Suitability to Various Regions

Since daily weather data and crop genetic coefficients are required for each cultivar/region plus a few soil properties, CERES-Maize is adaptable to most regions. CERES-Maize was modified and integrated into DSSAT (Decision Support System for Agrotechnology Transfer) by IBSNAT (International Benchmark Sites Network for Agrotechnology Transfer, Godwin *et al.*, 1989) to join a team of models for agrotechnology transfer.

Initial development of CERES-Maize was based on datasets of maize phenology, grain, leaf, dry matter, nitrogen concentration, and soil water data from many locations (Ritchie *et al.*, 1986). The nitrogen version has produced accurate simulations of the effects of N applications on biomass, total N uptake, grain N concentration and yield. CERES-Maize has been tested with many data sets from diverse location spanning the world's cropping regions since it was developed (Godwin *et al.*, 1984; Singh, 1985; Legowo, 1987; Carberry *et al.*, 1989; Ogoshi, 1995). Bowen *et al.* (1993) evaluated the CERES-Maize N version with measured data from a series of field experiments on an Oxisol in central Brazil from 1984 through 1987. They found that CERES-Maize had underpredicted N uptake by maize because of underestimating inorganic N in soil profiles. Assuming nitrate adsorption causes the problem, Bowen *et al.* (1993) improved the model's prediction in the case by including nitrate retention due to positive soil charge, a common phenomenon of acid tropical soils, which violated an initial assumption in the development of CERES-Maize.

3-6.4. Software & Hardware Environment

Written in Microsoft FORTRAN and distributed with sample input/output files, CERES-Maize source code can be modified by users. Jones and Kiniry (1986) provided extensive documentation of the model structure, input/output files, evaluation, and step-by-step operation instructions. CERES-Maize offers samples of input and output files as scenarios for users. As many simulation models, CERES-Maize provided no online help and almost no interactions with users during execution. When used within the DSSAT format, the model was supported for file saving menu selection and output analysis etc.

3-6.5. Conclusion

CERES-Maize is a dynamic mathematical model that simulates the biological and physical processes of maize growth and the nitrogen cycle in plant-soil systems. It is a very useful simulation model for professionals who need to predict the crop growth and N cycle in soil-plant systems for planning or agricultural technology transfer.

3-7. LEACHN: Deterministic Model for Simulating Nitrogen Dynamics in Soils

3-7.1. System Purposes

LEACHM, Leaching Estimation And CHemistry Models, is a set of process-based models of water and solute movement, transformation, plant uptake and chemical reactions in unsaturated soils (Wagenet and Hutson, 1989). LEACHN, the nitrogen version of LEACHM (other versions deal with water, pesticides, chemicals, and microbiology), is a deterministic model of simulating various chemical, physical and biological processes of nitrogen in soils (Hutson and Wagenet, 1991). The model uses a numerical solution of the Richards equation for water flow and the convection-dispersion equation for chemical transport in soils. LEACHN consists of independent subroutines for: 1) Water flow; 2) Chemical transport; 3) Evapotranspiration; 4) Heat flow; 5) Rate constant adjustment for temperature and water content; 6) Nitrogen transformation; 7) Plant growth; 8) Nitrogen uptake by plants. The main program of LEACHN initializes variables, performs mass balance calculations, and simulates different processes by calling the above subroutines.

3-7.2. System Inputs & Outputs

- **Inputs**

Required inputs include retentivity, hydraulic conductivity and dispersivity in the Richard equation and the convection-dispersion equation. Some suggestions (Hutson and Wagenet, 1991) can help users to estimate these data if they are not available. Main data inputs consist of:

1) **Soil physical properties** for each layer: water potential, hydrologic constants for moisture retentivity, hydraulic conductivity, texture, and bulk density.

2) **Crop data**: time of planting, dates of rooting, crop maturity and harvest, pan factor for crop evapotranspiration, and plant water potentials.

3) **Nitrogen and carbon data**: (a) Nitrogen and carbon contents in the profile, such as urea, ammonium, nitrate, humus, and manure; (b) N transformation parameters such as a synthesis efficiency factor, humification fraction, mineralization and nitrification rates; (c) Nitrogen and carbon applications.

4) **Weather and irrigation data**: amount of rainfall and irrigation (frequency and rate of water application), weekly pan evaporation, and mean temperature and amplitude.

- **Outputs**

Outputs consist of several tables of predicted data at specified time intervals for the soil profile:

1) Water retentivity (volumetric water content at several values of matric potential) and hydraulic conductivity.

2) A cumulative mass balance summary.

3) Chemical contents such as urea, NH_4^+, NO_3^-, litter-N/C, humus-N/C, and manure-N/C.

4) Plant growth, transpiration and nitrogen uptake.

3-7.3. System Suitability to Various Regions

LEACHN has been widely used in simulating nitrate transport in soils in many countries (Hutson and Wagenet, 1992). In Hawaii, LEACHN was successfully calibrated and predicted nitrate leaching from agricultural lands in response to fertilization, N transformation, climate and plant growth (Ling, 1996).

3-7.4. Software & Hardware Environment

LEACHN was written in FORTRAN. No installation is needed. Besides a diagram showing its structure, all mathematical equations were well documented in the manual. LEACHN provides example input files to assist users in entering data that conform to the FORTRAN format.

3-7.5. Conclusion

LEACHN was designed for soil scientists to predict nitrogen status in soil-water systems. The model is a good simulation tool for scientists but not for nonprofessionals. LEACHN worked well in simulating nitrate distribution in one dimensional flux pattern in unsaturated soils (Ling, 1996).

3-8. CENTURY: General Model of the Cycling of C, N, S, and P Through Organic Matter

3-8.1. System Purposes

The production and decomposition of organic material play an important role in the cycling of plant nutrients, influencing water relations, erosion potential, and soil structure. The CENTURY model was designed to simulate large-scale and long-term consequences of climate and management changes on C, N, P, and S dynamics in agroecosystems (Parton, *et al.*, 1987, 1988). Potential users of CENTURY are definitely scientists. CENTURY has been used to simulate carbon and nutrient (N, P, S) dynamics in different types of ecosystems (grasslands, forest, crop and savanna). The simulation can vary from a single year cycle to millennia.

3-8.2. System Inputs & Outputs

Major input variables include:

1) monthly average, minimum and maximum air temperature,
2) monthly precipitation,
3) lignin content of plant material,
4) plant N, P, and S content,
5) soil pH and soil texture,
6) atmospheric and soil N inputs,
7) initial soil C, N, P, and S levels.

Outputs consist of many dependent variables related to C, N, P, S and water, printed and plotted on the screen. CENTURY provides a program to help users initialize the model and adapt to site specific parameters. The site specific parameters include: model control parameters, ecosystems' specific management, initial plant production parameters, initial soil conditions, and other soil and weather data. If no local data available, input variables can be estimated from the literature or from expert consultations.

3-8.3. System Suitability for Various Regions

The model was validated against steady-state soil C and N levels and aboveground plant production for 24 sites in the Great Plains. Results showed that simulated plant production was highly correlated with simulated N inputs, which were direct functions of annual precipitation. The observed plant production was also highly correlated with annual precipitation. Results show that CENTURY can be adapted to various temperate regions.

3-8.4. Software & Hardware Environment

CENTURY consists of two major modules: a simulation program developed using FORTRAN and a graphic display program VIEW (a commercial module of TIME-ZERO). CENTURYM saves simulation results for VIEW to output as plots or tables. Users can plot or print more than 170 CENTURY variables using VIEW. The manual provides charts and diagrams to show model structures and examples for input data. The space required for output files varies with simulation years. For example, a 100-year simulation with monthly data requires about 2 MB of disk space.

3-8.5. Conclusion

CENTURY is a strong model for predicting a long term cycling of C, N, S, and P contained in organic materials, but is nearly inaccessible to nonprofessionals because of its extensive use of technical jargon. Scientists who work on large scale ecosystems such as agro-forestry systems in an agricultural region may find CENTURY useful.

3-9. TORBERT '93: Simulation of Soil-Plant Nitrogen Interactions for Educational Purposes

3-9.1. System Purposes

TORBERT '93 was designed as a teaching tool for the classroom rather than as a research or management tool. It can help students understand the complex dynamic processes associated with physical, biological, and chemical components of the N cycle in soil-plant systems (Torbert, *et al.*, 1994). The model simulates water, C, and N changes in the various N pools over a time span of one year under certain climatic factor interactions. Mass flows between pools are controlled by reaction components using chemical reaction equations. TORBERT '93 was designed for three levels of users: beginning, medium, and advanced. The beginner can use the system by inputting data and comparing output for general concepts of the N cycle in soil-plant systems. Advanced users can examine each component of the system at the programming level and modify the system with their ideas.

3-9.2. System Inputs & Outputs

Inputs are set in the "scenario" section, where TORBERT '93 provides users with 15 choices that establish conditions for the simulation. These choices are related to rainfall, temperature, fertilization, planting date, expected corn yield, and soil type. There are 133 dependent variables as model outputs in three categories: 1) 18 "stock" variables that accumulate flows of material and energy (e.g., soil adsorbed ammonium, soil solution ammonium, soil nitrate, and N in growing plants); 2) 26 "*flow*" variables that fill and drain "*stock*" variables (e.g., the plant uptake N per unit period, the nitrification rate of ammonium, the mineralization rate of organic N, and the adsorption rate of ammonium); and 3) 99 "*converter*" variables that serve utilitarian roles as constants (e.g., conversion rates and fractions), external inputs (e.g., fertilizers), or as algebraic relationships (e.g., equations). Outputs are simulated N in various pools changing with time. Users can monitor the consequences of the cycle of selected variables in graphical or tabular outputs during the simulation.

3-9.3. System Suitability for Various Regions

As a teaching tool, TORBERT '93 was apparently not designed for research or extension in the current version. No validation was documented. Most model parameters and default data were from the literature.

3-9.4. Software & Hardware Environment

TORBERT '93 was developed with STELLA II, a model developmental shell (Peterson and Richmond, 1994). STELLA II provides TORBERT '93 with an impressive and easy-to-use graphical interface for constructing the model. STELLA II simulation environment allows users to easily examine model structure from three scales: 1) an overall model map, 2) an overall model construction, and 3) sub-models. Like most systems developed using shells, TORBERT '93 can be modified at runtime in structures, equations and parameters by users. Users can learn STELLA II using the accompanying tutorial and easily modify the model in many ways. In other words, TORBERT '93 is easily upgraded or revised as long as users have access to the STELLA II development shell.

3-9.5. Conclusion

TORBERT '93 is a good example of an N cycle description that was constructed using a modeling shell with visual programming. The model is an attractive teaching tool to learn the N cycle in classrooms with scenarios.

3-10. Summary

Nine N models were summarized in Table 3-10.1. Among the models, NDSS, QUEFTS, and NITROP were used for calculating the requirement of N fertilizer and economic evaluation. NLEAP and AGNPS were designed as environmental assessment tools: NLEAP predicts nitrate leaching to groundwater while AGNPS deals with surface water quality. These systems describe the N budget among soils, crops, atmosphere, and water. The remaining systems are dynamic simulation models that describe and predict the N cycle between soils and plants in agroecosystems. CERES-Maize (N version) simulated corn growth and the N cycle in the maize-soil system. LEACHN predicts N leaching in soil profiles at specific intervals. CENTURY was constructed for long-term predictions of agroecological regions. TORBERT '93 simulates the N cycle for education purposes.

These models described current knowledge and techniques of modeling the N cycle in soil-plant systems and were suitable for static estimation, dynamic simulation, assessment, and general planning. However, they were weak at dynamic optimization and modeling management actions (e.g., specific timing fertilization and irrigation), especially for in-season management. To optimize N management for maximizing productivity, economic values, while eliminating the environmental impact, the "gaps" in modeling N management activities must be filled by further development.

Table 3-10.1. Evaluation Summary of Nitrogen Models

	NDSS	QUEFTS	NITROP
MODEL TYPE	calculation model	simulation, calculation model	expert system, calculation
DEVELOPER	Reid, Shaw, et al.	Janssen, B.H., et al.	Deanna Lynn Osmond
	Cornell University	University of Wageningen	Cornell University
DEVELOPED DATE	Nov. 1992	Mar. 1990	Jan. 1991
MODEL DESCRIPTION			
Objectives	determine N fertilizer requirement	determine N, P, K fertilizer requirement	determine N fertilizer requirement
Problems to be solved	N fertilizer application	N fertilizer application	N fertilizer application
Potential users	farmers	farmers	farmers
Required education levels	high school	high school	high school
Benefits from the system	economic	economic	economic
Major limitations	assumption of N deficiency only	assumption of N deficiency only	assumption of N deficiency only
INPUTS & OUTPUTS			
Major inputs	crops, soils, manures	crops, soils, climate	crops, soils
Major outputs	amount of N fertilizer to apply	amount of N, P, K fertilizers to apply	amount of N fertilizer to apply
Data management	dBASE	model files	from keyboard
Minimum input variables	40	40 - 50	12 - 15
Data collection	from users	from users	from users
Data properties	quantitative	quantitative	quantitative/qualitative
Default situations	default databases	default files	in the program
SOFTWARE			
Developing tools	Foxpro 2.0	Turbo Pascal 5.0	VP-Expert
Interface	Foxpro specific	DOS program	VP-Expert shell
Examples, Tutorials	DEMO data sets	examples	no
Manual, Readme files	no Readme files	user guide (hard copy)	manual (hard copy)
Software requirement	DOS 3.x or greater	DOS 3.x or greater	DOS 3.x or greater
Hardware requirement *	IBM: RAM 640K, disk 2.4 M	IBM: RAM 512K, disk 1.3M	IBM: RAM 384K , disk 704K

* Disk refers to floppy or fixed. Space only for the package, not for working space.

Table 3-10.1. (continued) Evaluation Summary of Nitrogen Models

	NLEAP	AGNPS	CERES-Maize (N version)
MODEL TYPE	computation model	frame work with maps	simulation model
DEVELOPER	Shaffer, M.J., et al.	Yong, R.A., et al.	Ritchie et al.
	USDA-ARS	USDA-ARS	USDA-ARS et al.
DEVELOPED DATE	1991	July 1991	June 1986
MODEL DESCRIPTION			
Objectives	predicting leaching risk	assessment of pollution	predict N dynamics
Problems to be solved	nitrate leaching to groundwater	pollution of surface water	N dynamics in corn -soils
Potential users	action and extension agencies	scientists, action agencies	scientists, action agencies
Required education levels	college	college	college
Benefits from the system	environment	environment	production & environment
Major limitations	qualitative estimates	qualitative estimates	assumption of regular agro. condition
INPUTS & OUTPUTS			
Major inputs	soils, precipitation, hydrology, cropping	runoff, sediment, N & P nutrients	crops, soils, management, weather
Major outputs	prediction of nitrate fate	prediction of water quality	simulation tables for N & corn data
Data management	model databases	model databases	simple ASCII files
Minimum input variables	80 - 95	depends on acre to assess	40-60 plus weather data
Data collection	from users, testing, database	from users, testing, database	from users, literatures, database
Data properties	quantitative/qualitative	quantitative	quantitative
Default situations	parts of default inputs	no default inputs	parts of default inputs
SOFTWARE			
Developing tools	MS C, Fortran 77	Fortran 77	MS Fortran
Interface	DOS program	DOS, maps	DOS program
Examples, Tutorials	no examples	example data sets	example input/output files
Manual, Readme files	Readme files, articles	user guide, but no Readme files	publication (hard copy)
Software requirement	DOS 3.x or greater	DOS 3.x or greater	DOS 2.0 or greater
Hardware requirement *	IBM: RAM 640K, disk 3M	IBM: RAM 640K, disk 1.4M	IBM: RAM 256K, disk 720K

* Disk refers to floppy or fixed. Space only for the package, not for working space.

Table 3-10.1. (continued) **Evaluation Summary of Nitrogen Models**

	LEACHN	CENTURY	TORBERT
MODEL TYPE	simulation model	simulation model	simulation model
DEVELOPER	Hutson and Wagenet	Parton, W.J. et al.	Torbert, H.A., et al.
	Cornell University	Colorado State University	USDA-ARS
DEVELOPED DATE	1987 -1992	1992	1993
MODEL DESCRIPTION			
Objectives	predicting N leaching	long-term prediction	teaching tool
Problems to be solved	N leaching on soil profile	cycle of C, N, S, P simulation	soil-plant N simulation
Potential users	scientists, action agencies	scientists	students
Required education levels	college	college	high school, college
Benefits from the system	environment	science	education
Major limitations	for water, chemicals leaching only	Scientific data search	the parameters from literature
INPUTS & OUTPUTS			
Major inputs	hydrology, soils, weather, crops	climate, crops, soils	plants, soils
Major outputs	simulation tables for N & soil water	simulation plots, tables for C, N, P, S	simulation plots (or tables) for N
Data management	simple ASCII files	ASCII files	parameters in the model
Minimum input variables	40 plus 30 * soil layers + 4 * weeks	195	15 choices in scenarios
Data collection	from users, testing, database	from users, literatures	from users, literatures
Data properties	quantitative	quantitative/qualitative	quantitative/qualitative
Default situations	parts of default inputs	default files	in the program
SOFTWARE			
Developing tools	Fortran	Fortran , TIME-ZERO	Stella II
Interface	DOS program	DOS, TIME-ZERO	Windows, graphic
Examples, Tutorials	example input/output files	sample data sets	no examples, tutorials from shell
Manual, Readme files	manual (hard copy) & readme	manual (hard copy)	manual for shell
Software requirement	DOS 3.x or greater	DOS 3.x or greater	MS Windows, Stella II
Hardware requirement *	IBM: RAM 640K, disk 1.4M	IBM, RAM 512K, disk 614K	IBM, MAC: model 357K , shell 2.7M

* Disk refers to floppy or fixed. Space only for the package, not for working space.

Chapter 4

Dynamic Nitrogen Model

Some preliminary experiments to improve N models in management were documented in a static N model, *N-Balance for Windows* (Yost *et al.,* 1997a). Although the static N model can estimate overall nitrogen budgets of soil-crop systems during a cropping season, it does not evaluate nitrate leaching precisely because leaching is a dynamic process partially determined by rain events. The static model is also weak in predicting the influences of human management related to the amounts and timing of N application and irrigation on nitrate leaching. A dynamic model is needed for these estimates. In an overview of numerical models for nitrate leaching, Ling (1996) categorized the deterministic models' approach into two groups. The first approach uses the numerical solution of the convection-dispersion equation (CDE) and the second approach applies the mass balance method. The mass balance approach has been widely applied in modeling N in soil-plant systems (CERES-Maize, Jones and

Kiniry, 1986; CENTURY, Parton *et al.*, 1988; SOYGRO, Jones *et al.*, 1991b; Torbert '93, Torbert *et al.*, 1994). This method was used to construct the dynamic model in this study because it can provide information of N and water in diverse pools and forms, which is needed in Management-Oriented Modeling (See Chapter 5). In the whole system of Management-Oriented Modeling, the dynamic model is only a component that plays the role of a simulator, even though it can be used as an independent N simulation model. Therefore, the dynamic N model to be developed in this chapter is called N-SIMULATOR.

4-1. System Definitions

Before describing the model, the goals and boundaries of the model was defined below with assumptions and declarations for whom and for what tasks the model is designed.

4-1.1. Goals of the Model

1. The model described here was designed as a tool that assists users to make decisions on N fertilizer management during a cropping season. Potential users of the model include agronomists, teachers, researchers, agricultural extension agents, consultants, government action agents, farmers, land owners and managers, and others who are involved in crop and soil management.
2. The model should require the least amount of data, for example, standard soil and plant tissue test data, data from currently available soil and weather databases, or the data that users can easily obtain.

3. The model should provide users with a dynamic picture of the N cycle that includes the N uptake by a plant, N remaining in the soil profile, and nitrate leaching out of the root zone during a cropping season. These dynamic data are important for users to minimize nitrate leaching and maximize crop production and profits.

4. Technologically, the model should contain the necessary N components while making the structure simple to run as fast as possible. The model is implemented as a simulator in Management-Oriented Modeling (See Chapter 5), which requires that the model simulate the N cycle in soil-plant systems for an entire cropping season in a few seconds. For example, simulating nitrogen transformations, crop uptake, nitrate leaching, and water movement in a whole soil profile for 120 days of cropping should finish in 1-2 seconds on currently available personal computers (e.g., 66-100 MHZ PC).

4-1.2. Boundaries of the Model

To understand where the model may be applicable and what tasks the model is designed to perform, the boundaries of the model must be clearly defined in spatial and time dimensions. These boundaries are defined below.

4-1.2.1. Spatial Dimension

Based on the goals of decision-aid for cropping and fertilization management, the model is designed as a **field-scale** system that describe a whole-crop system.

In the **horizontal** dimension, the system boundaries are set by the area of **a field** with the same soil type (or similar soil properties). The fields are basic management units for farmers and most fertilization practices. For a watershed, a field looks like a polypedon (Fig. 4-1.1.). Therefore, the model would partially work for a watershed when it is running simultaneously for all fields in the watershed.

In the **vertical** dimension, the system boundaries are from the top of a crop to the bottom of the root zone. Because most important nitrogen transformation activities take place in the root zone, we divide the soil profile of the root zone into three horizons: **major root zone, minor root zone** and **transition zone** (Fig. 4-1.2.). The

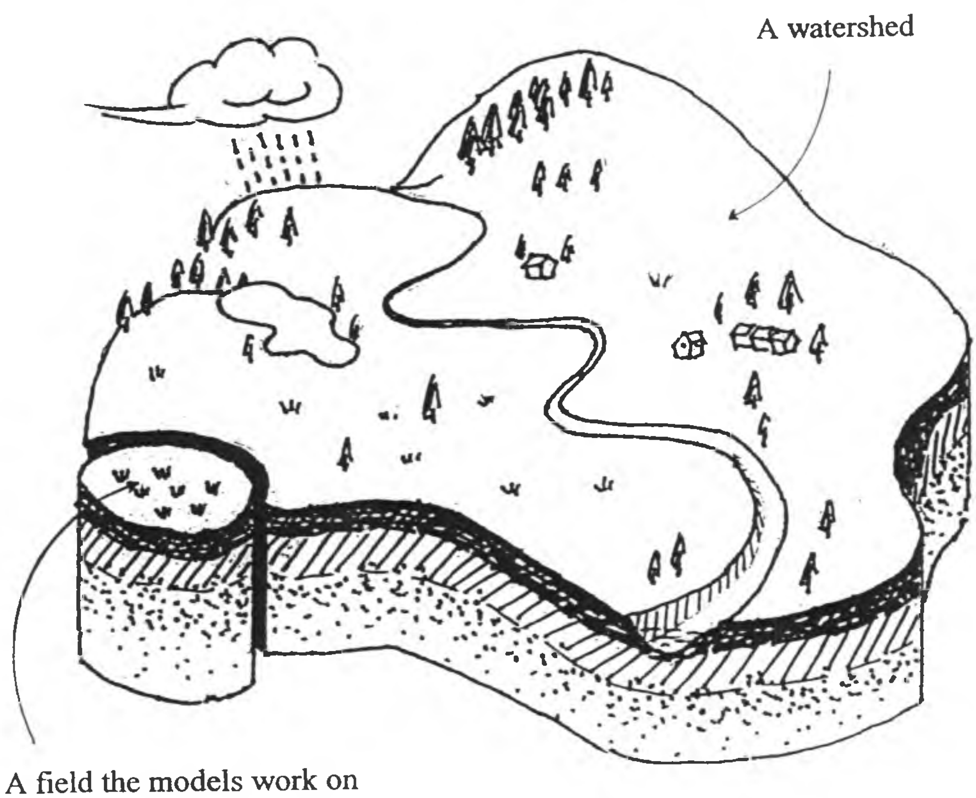

Fig. 4-1.1. The system horizontal boundaries of the model is around an area of a **field** with the same soil type (or similar soil properties). The field that the model works on looks like a polypedon in a watershed. Fields are often basic units of agricultural activities and management.

major root zone is the soil surface layer where crops usually develop the majority of their root systems. This layer is also the major zone for additions of fertilizers and water, plant uptake, N transformations, and surface evaporation. The minor root zone has less root density and less organic N mineralization associated with soil microorganisms. This zone plays a smaller role in N uptake by plants but an important

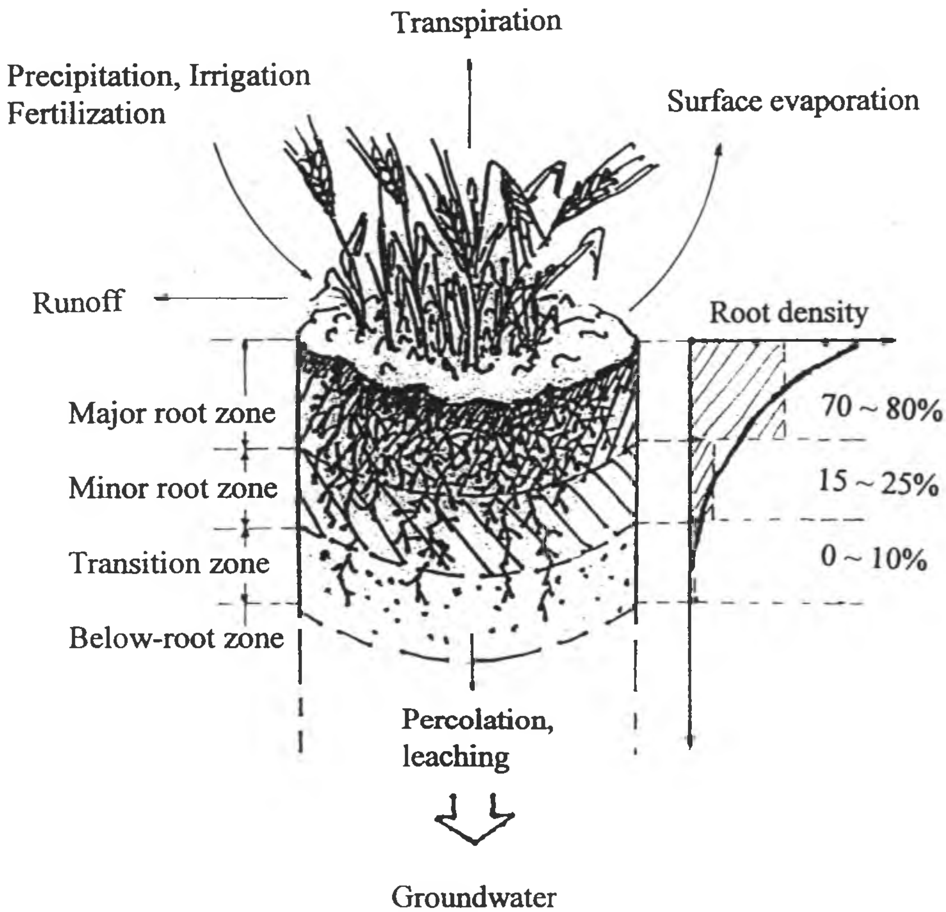

Fig. 4-1.2. In the vertical dimension, the system boundaries of the model is from top of a crop to bottom of the root zone. The soil profile of the root zone is divided into three horizons: **a major root zone, a minor root zone and a transition zone**. After N and water are applied to the soil, N transformations are simulated within the layers, and water and N movement is simulated across the layers. Nitrate moved to the below-root zone is considered leached out of the root zone.

role in nitrate leaching. The transition zone is defined as the zone in which the root fraction is less than 10%. Only a small fraction of inorganic nitrogen (nitrate in most uplands) in this zone can be utilized by plants. Potential nitrate leaching may occur in this zone unless subsequent crops can develop more roots into this zone. This division is helpful to estimate dynamic N transformations, crop uptake, and nitrate leaching without requiring extra data other than routine soil tests. With soil test data from the major root zone, the soil data of the minor root zone and transition zone can be estimated using soil databases and/or local experimental data. These estimates should be acceptable in most situations for two reasons. First, the main soil N comes from the soil organic N source that is approximately 80% of total N (Yost, 1992). So the majority of soil N, the organic N, below the major root zone can be estimated from the distribution of organic N (associated with soil organic carbon) in soil profiles. The distribution patterns of soil organic C (or organic N) in the soil profile can be described by soil test results or be derived from soil databases or soil surveys (SCS-USDA *et al.*, 1976). Second, errors in estimating the N uptake from a minor root zone and transition zone have a small influence on whole N uptake because there are small portions of root densities, organic N contents, and microorganism activities in the minor root zone and transition zone, compared to those in the major root zone. Assuming 20% of the roots are in the minor root zone, 5% are in the transition zone, and 20% of the soil N is derived from soil inorganic N, for example, the maximum estimating error in the N uptake is 5% (20% · 25%), without artificial fertilizers. This error will be further reduced when applying a certain amount of fertilizer. For instance, if 50% of the uptake N comes from the applied fertilizer, the error of estimating the N uptake from soil N in the minor root zone and transition zone will decrease from 5% to 2.5%, in the example above.

Each root zone, however, can be further divided into a number of sub-layers that will increase simulation precision, provided there is sufficient soil profile data. This is very useful for the systems used in scientific research and in some specific applications that need to simulate more soil layers.

4-1.2.2. Time Dimension

A model time step refers to the period of time to complete one cycle of the model session. This period of time is also associated with the frequency of data input. Generally, model time steps associated with cropping are determined by crop types, cropping systems, and the management goals. Long time (several years or more) steps are often used for perennial crops or rotational cropping systems. Some management objectives require decades or centuries as time steps (Parton, et al., 1987, 1988). A one-year time step or one crop growing season time step is often used for annual crops or model objectives related to a growing season basis (Seligman and Keulen, 1981; Jones *et al.*, 1984; Ritchie *et al.*, 1986). The **time steps** of the model in this study were limited to **one cropping season** for a running session which include weekly and daily simulation steps. These time steps reflect a basic time unit of management for most agricultural crops. If model initial states are based on the test or observed data, shorter time steps have lower risks of making errors in prediction than a longer one at the same modeling precision.

4-1.3. Critical Assumptions

Crops

The model is designed for annual or perennial upland crops. If there are other crops (including weeds) in the fields, their N uptake must be a very small fraction that can be ignored compared to that of the major crop. The crop should have no severe problems of pests, diseases, macro- or micro-nutrient deficiencies except nitrogen. It is also supposed that crop roots develop normally. In other words, the model does not consider the effects of soil chemical and physical barriers or enhancements on root development.

Soil

The model assumes that soil physical and chemical properties within a layer (e.g., one of the root zones) are homogeneous in horizontal and vertical dimensions. These properties include hydraulic conductivity, water content, bulk density, nutrient content, pH, and other properties such as nitrate adsorption. It is further assumed that there are no significant coarse fragments or lithic horizons, duripans, or fragipans in the root zone and immediately below the root zone, which may significantly slow vertical root penetration and water movement. The water table is assumed to be far below the root zone and to have no influence on the soil water movement in the root zone. Any nutrients moving out of the root zone into the below-root zone (Fig. 4-1.2) are assumed not to be absorbed by crops. Nitrate in the below-root zone is all allocated to potential leaching if the next crops in the following cropping season cannot penetrate their roots into this horizon.

Weather

Normal local weather conditions prevail for crop growing in a modeling session.

Management

The model is supposed to run under a good or a normal agronomic management practice in local conditions. Most model coefficients should be adapted to local conditions by users, perhaps with assistance from local experts (See Appendix C). However, some management strategies such as the amounts and frequencies of irrigation and N fertilization are designed as variables in Management-Oriented Modeling (See Chapter 5), which are solved by the model.

4-2. Nitrogen Cycle Modules

4-2.1. Nitrogen Cycle in Ecosystems

Nitrogen is involved in cyclical transformations of four major global compartments in the biosphere: atmosphere, water, living organisms, and soil (Sprent, 1987).

1. **Atmosphere**

   The major nitrogen component in the atmosphere is the dinitrogen molecule, N_2, which makes up about 79% of the atmosphere. The second form includes nitrogen oxides such as N_2O (nitrous oxide), NO (nitric oxide), and NO_2 (nitrogen dioxide). The third form is reduced nitrogen that contained in ammonia (main form) and various organic compounds.

2. Water

The main components of nitrogen in this compartment are dissolved nitrogen gases. There are also low concentrations of ammonia, urea, and some low molecular weight organic compounds.

3. Living Organisms

Nitrogen is one of the most important elements in living organisms. It is present in various forms in the cell: gas, solution in both oxidized and reduced forms.

4. Soil

All forms of nitrogen listed above may exist in soil. In addition to organic N compounds, ammonium and nitrate are major inorganic forms in soil.

Many diagrams of the N processes have been used to show the nitrogen cycle from different standpoints and for different purposes. For example, if we are interested in soil-plant systems, a conceptual view of the internal N cycle may be useful (Fig. 4-2.1.). The internal N cycle is operative in soil distinct from the overall cycle of N in nature but interfaces with it (Stevenson, 1985). To develop a dynamic model to assist N management, the modeling would mainly focus on the **nitrogen cycle within the soil** root zone, not modeling the nitrogen transformations in plant cells. Although it is impossible to model all physical, chemical, and biological processes of the nitrogen cycle in soil, the most significant factors and processes will be considered in model. Fig. 4-2.2 shows main processes of the N cycle in N-SIMULATOR. The discussion of

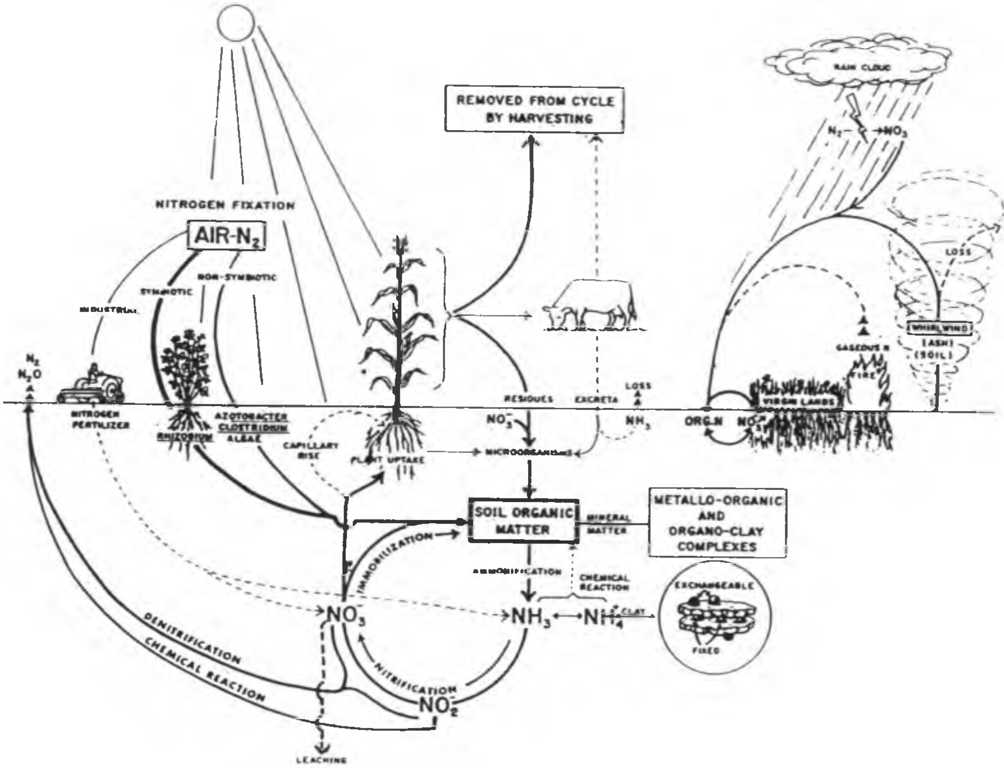

Fig. 4-2.1. A conceptual view of the internal N cycle in soil-plant systems. Source: Stevenson, F.J. (1985).

the following sections will focus on how the model simulates these processes, not the mechanisms of these processes.

4-2.2. Soil Moisture and Temperature Factors

The major nitrogen transformations in the soil root zone simulated in N-SIMULATOR are urea hydrolysis, ammonia volatilization, mineralization, immobilization, nitrification, and denitrification. These processes are significantly affected by soil moisture and temperature and some of those are also sensitive to soil

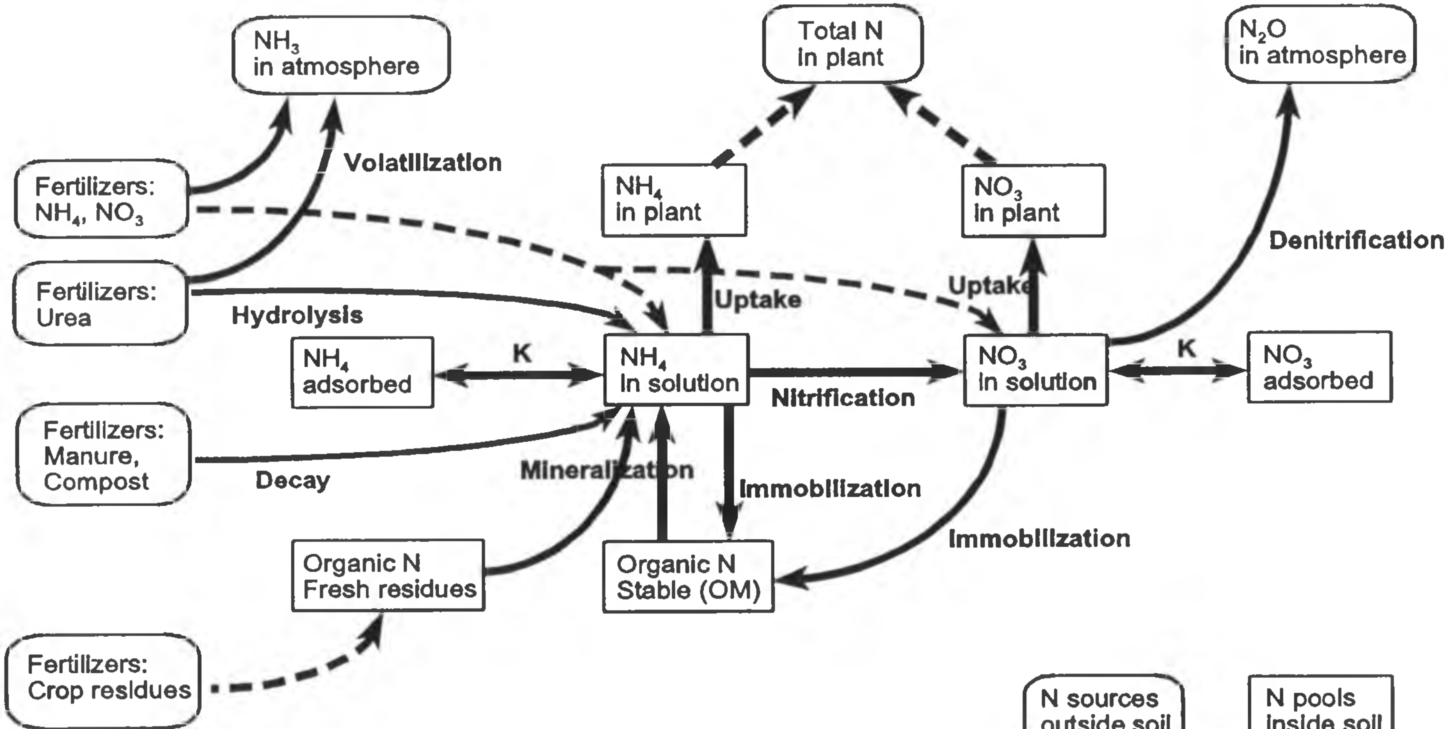

Fig. 4-2.2. Main processes of nitrogen transformations in the dynamic model.

pH and other factors. To represent the influences of these environmental factors on the processes, indexing or rating function was commonly used in various models (Hackett, 1991; Jones *et al.*, 1991; Godwin and Jones, 1991; Shaffer *et al.*, 1991; Torbert *et al.*, 1994). These functions are used when more detailed functions are not yet known in our current knowledge. Examples of such functions are 0-1 index functions used to adjust the influences of soil moisture and temperature on main N processes in N-SIMULATOR (Fig. 4-2.3 and Fig. 4-2.4). These function values were mainly derived from the CERES-N model (Jones and Kiniry, 1986), Torbert '93 model (Torbert *et al.*, 1994), SOYGRO model (Jones *et al.*, 1991b), and NLEAP model (Shaffer *et al.*, 1991). Unless indicated otherwise, the functions and coefficients of soil nitrogen transformations in N-SIMULATOR were mainly drawn from these models. In moisture adjustments (Fig. 4-2.3), the term *PlantLmt* is defined as the lower limit of plant extractable soil water content (LL in CERES-N model); *DrainLmt* refers to soil water content at the drained upper limit (DUL in CERES-N model); and *SaturatLmt* refers to the content at saturation (SAT in CERES-N model, Jones and Kiniry, 1986). N-SIMULATOR implements these concepts from the water balance module of CERES-N, which have been successfully validated (Jones and Kiniry, 1986; Legowo, 1987; Ritchie *et al.*, 1989; Tsuji *et al.*, 1994). This borrowing saves the time and effort in finding soil water coefficients and corresponded validation because CERES-N has accumulated many methods to estimate soil water coefficients. Soil nitrogen transformation rates are strongly affected by environmental factors such as soil moisture, temperature, and pH. Referring to Liebig's "law of the minimum" (Liebig,

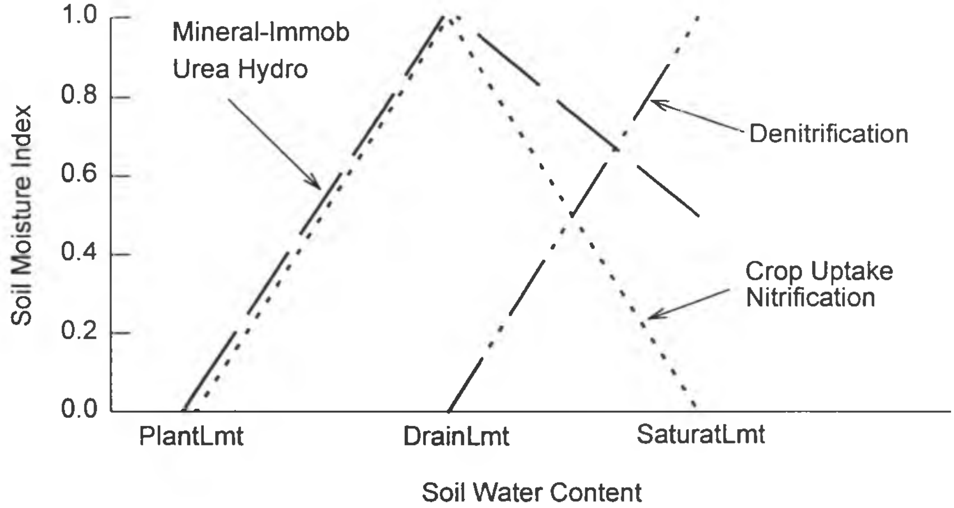

Fig. 4-2.3. Soil Moisture Index used to adjust N transformation rates and crop N uptake. Derived from CERES-N model (Godwin and Jones, 1991), Torbert '93 model (Torbert et al., 1994), and NLEAP model (Shaffer et al., 1991).

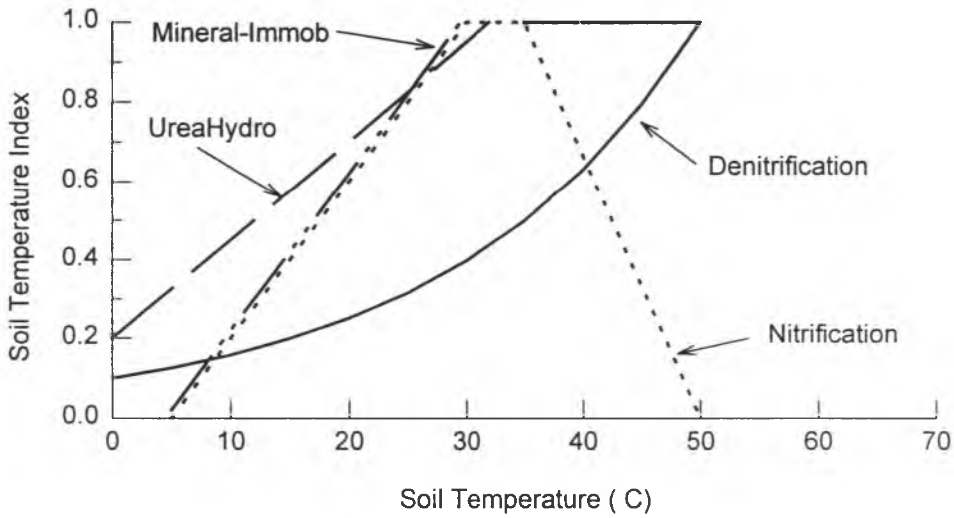

Fig. 4-2.4. Soil Temperature Index used to adjust N transformation rates. Derived from CERES-N model (Godwin and Jones, 1991), Torbert '93 model (Torbert et al., 1994), and NLEAP model (Shaffer et al., 1991).

1855), the most limiting factor among the factors plays a key role in restricting N transformation rates. The factor that most limits nitrogen transformation rates is selected using the following function:

$$Rate_{Actual} = SelectMin\ (F_{moisture}, F_{temperature}, F_{pH}, \ldots) \cdot Rate_{Max} \qquad [4\text{-}2.1]$$

where *SelectMin* is a function that returns the minimum of a list of terms. CERES-N model implements this approach in many processes (Godwin and Jones, 1991). The adjustment of other environmental factors will be discussed individually.

4-2.3. Urea Hydrolysis and Ammonia Volatilization

The sources of urea and ammonia and/or ammonium may be commercial fertilizers and organic wastes such as animal manures. When fertilizers and solid organic wastes are applied, N-SIMULATOR assumes they are uniformly incorporated into the soil surface layer (the major root zone) and accumulated in the pools of urea and ammonium (Fig. 4-2.2). The two processes in N-SIMULATOR, urea hydrolysis and ammonia volatilization, begin when fertilizers or organic wastes are applied.

Urea Hydrolysis

Khan *et al.* (1986) modeled the processes of urea ⇒ ammonium ⇒ nitrate using first-order kinetic equations. To determine transformation rates for the nitrogen model, they conducted experiments on an Oxisol (*clayey, kaolinitic, isohyperthermic Tropeptic Eutrustox, Wahiawa series*). The model successfully fit the experimental data. Khan *et al.* noted that urea hydrolysis and other N transformation rates varied with environmental factors such as pH, temperature, and moisture. To relate the environmental factors to the rates, CERES-N model (Godwin and Jones, 1991) uses an equation to determine the maximum urea hydrolysis rate for each soil layer:

$$Rate_{Max} = -1.12 + 1.31C_{Hmc} + 0.203\,pH - 0.155C_{Hmc}\,pH \qquad [4\text{-}2.2a]$$

where $Rate_{Max}$ is a maximum urea hydrolysis rate (day^{-1}), C_{Hmc} is the humic soil organic carbon (%), and pH is soil pH (H_2O). This maximum urea hydrolysis rate was estimated from several laboratory studies (McGarity and M.G.Myers, 1967; Myers and McGarity, 1968; Tabatabai and Bremner, 1972; Zantua *et al.*, 1977). The actual urea hydrolysis rate was derived from adjusting the maximum rate by soil temperature and moisture (Vleck and Carter, 1983). The urea hydrolysis rate in N-SIMULATOR is calculated by equation [4-2.2a]. The soil moisture and temperature influences on the urea hydrolysis rate are adjusted by equation [4-2.1] and the unification factors shown in Fig. 4-2.3 and Fig. 4-2.4.

Ammonia Volatilization

Ammonia volatilization loss is estimated when N fertilizers or organic wastes that contain ammonia (or ammonium) are applied. N-SIMULATOR uses the equations and coefficients used in N-BALANCE model (Yost *et al.*, 1997a) except for the maximum volatilization rate. Daily fraction of fertilizer volatilization, Fv_{fert}, is calculated by

$$Fv_{fert} = Fv_{pH} \cdot Fv_{temp} \cdot K_{method} \cdot Fv_{max} \qquad [4\text{-}2.2b]$$

where, Fv_{pH} is a fertilizer volatilization loss fraction due to high soil pH (0-1). Fv_{temp} refers to a fertilizer volatilization loss fraction due to soil temperature (0-1). K_{method} means a volatilization coefficient of the application method (0-1). Fv_{max} is a maximum volatilization fraction for the worst application method/timing (0-1), which values are less than those in N-BALANCE model, because they are accounted for on a daily basis here while there is only one estimate for a whole cropping season in N-BALANCE model (Yost *et al.*, 1997a). Based on the estimated ammonium content in the major root zone, N-SIMULATOR simulates the volatilization loss in the first 10 days after fertilizers or organic wastes that contain ammonia (ammonium) or urea is applied. This is because approximately 90% of volatilization losses of fertilizer ammonia occur in first 10 to 15 days after the fertilizers are applied (Fox *et al.*, 1996).

4-2.4. Mineralization and Immobilization

It is well established that nitrogen mineralization in soils is a biological decomposition process in which organic nitrogen is converted into inorganic forms. Immobilization refers to the biological conversion of inorganic nitrogen (NH_4 and NO_3) into soil microbial tissue, reducing the amount of N available for immediate plant utilization (Fig. 4-2.2). Soil temperature and moisture are major factors controlling these processes. Since soil organic matter provides energy for the processes, the ratio of carbon to nitrogen (C/N) in soil organic matter determines the net effects of the two processes. In N-SIMULATOR, the mineralization (decomposition) of organic nitrogen is divided into two processes: mineralization of soil organic matter and decomposition of organic N waste materials such as animal manure (Fig. 4-2.2).

Mineralization of Soil Organic Matter

In the early 1980s, PAPPAN model successfully simulated mineralization-immobilization processes in annual pasture production systems (Seligman and Keulen, 1981). The soil organic matter source in PAPPAN was divided into two pools: 1) fresh organic matter such as crop residues and green manure, and 2) humic or stable organic matter. Based on PAPPAN model, CERES-N constructed its mineralization-immobilization modules with many modifications (Godwin and Jones, 1991). For example, CERES-N separated fresh organic pool into three sub-pools: carbohydrate (20%), cellulose (70%), and lignin (10%). This modification probably improves the estimation of denitrification in which soluble carbon is used. The CERES-N approaches of mineralization-immobilization matched our goals, therefore, N-SIMULATOR inherited CERES-N functions and coefficients of mineralization-immobilization to simulate the mineralization-immobilization of soil organic matter.

Decomposition of Organic Wastes

In N-SIMULATOR, organic wastes are categorized to three independent pools: (1) crop residues and green manure, (2) concentrated organic wastes such as animal manure, and (3) irrigation with diluted wastes. Crop residues and green manure are allocated to the fresh pools of soil organic matter. When crop residues or green manure is added, the soil C/N ratio of the surface layer changes. This change immediately affects soil mineralization-immobilization in the soil. When large amounts of crop residues with high C/N ratios are incorporated into soil, they cause a temporary shortage of inorganic nitrogen available to plants.

The second pool is designed for concentrated organic wastes, such as animal manure, that may not follow the linear mineralization rates. For this kind of organic materials, a first-order mineralization equation is employed in N-SIMULATOR to estimate their decomposition (Stanford and Smith, 1972):

$$N_t = N_p(1 - e^{-kt}) \qquad [4\text{-}2.3a]$$

where N_t is the cumulative amount of nitrogen mineralized at time t, N_p is the initial organic nitrogen that is potentially mineralizable, and k is mineralization rate constant. Using equation [4-2.3a] with various k, N-SIMULATOR simulates several organic wastes in parallel with different mineralization rate constants. This provides alternatives for simulating applications of multiple types of organic wastes during a cropping season.

For the irrigation with diluted organic wastes, mineralization rates may vary with the source of the waste. N-SIMULATOR reserves an independent pool in the first soil layer to store the organic N from waste irrigation. The daily mineralized NH_4 from this pool is estimated by

$$NH_4 = F_{Water} \cdot F_{Temp} \cdot K_{decay} \cdot N_{wstOrg} \qquad [4\text{-}2.3b]$$

where NH_4 *(kg N ha^{-1})* is ammonium decayed from the pool of organic N from waste irrigation, F_{Water} and F_{Temp} are soil moisture and temperature factors (Fig. 4-2.3 and Fig. 4-2.4), K_{decay} is the daily mineralization rate, and N_{wstOrg} *(kg N ha^{-1})* is the pool of organic N from waste irrigation in the first soil layer.

4-2.5. Nitrification and Denitrification

Nitrification is the oxidation of ammonium to nitrate while denitrification is the reduction of nitrate or nitrite to gaseous nitrogen such as N_2O, NO, and N_2. Microorganisms play important roles in the two processes. Nitrification usually occurs under aerobic condition while denitrification take places under anaerobic conditions. In addition to soil aeration, soil temperature and pH are important factors that limit these processes (Focht and Verstraete, 1977). CERES-N modified the Michaelis-Menten function described by McLaren (1970) to estimate nitrification rate $Rate_{Nitrification}$:

$$Rate_{Nitrification} = Factor_{MinLimit} \cdot \frac{40 \cdot C_{NH_4}}{90 + C_{NH_4}} N_{NH_4} \qquad [4\text{-}2.4]$$

where, $Factor_{MinLimit}$ is the minimum factor among factors of soil moisture, temperature, pH, and nitrification potential, C_{NH4} *(ppm)* is the ammonium concentration and N_{NH4} *(kgN ha^{-1})* is ammonium content. The function [4-2.4] is used in N-SIMULATOR to calculate nitrification rates, but constant 40 in equation [4-2.4] was changed to a variable that users can use to calibrate for local conditions.

The basic denitrification functions and coefficients in the CERES-N model were adapted from the studies of denitrification affected by irrigation frequency of a field soil (Rolston *et al.*, 1980). Rolston *et al.* (1984) also contributed the functions and coefficients to the Torbert '93 model. The function to estimate a daily denitrification rate in N-SIMULATOR is adopted from CERES-N model:

$$Rate_{denitrification} = 6 \cdot 10^{-4} \cdot F_{Water} \cdot F_{Temp} \cdot C_{SolubleCarbon} \cdot N_{NO3} \qquad [4\text{-}2.5]$$

where, $Rate_{denitrification}$ is the denitrification rate *(kgN ha^{-1} day^{-1})*, N_{NO3} is soil nitrate content *(kgN ha^{-1})*.

4-2.6. Plant Uptake

Model objectives determine the methods of simulating soil N uptake by crops. For example, genetic coefficients are important for SOYGRO, CERES-Maize, and CERES-Wheat models (Ogoshi, 1995). This is because CERES models were designed to simulate crop phenological development, growth, and yield (Jones *et al.*, 1984). For instance, SOYGRO was a phenology model used to predict soybean growth and yield (Jones *et al.*, 1991b). In CERES models, the process of plant N uptake was in connection with genetic coefficients of the plant species. The process was controlled by the differences between critical N concentration in plant tissue (related to plant phenological age) and current actual plant N concentration. In other words, CERES models use phenological rather than chronological age to determine crop uptake nitrogen (Godwin *et al.*, 1984).

N-SIMULATOR is not a crop growth model with the same purposes as above models. N-SIMULATOR is only designed to describe how much N a local crop can actually accumulate under local conditions. This is estimated from crop maximum uptake rates under local conditions, adjusted by environmental factors rather than genetic coefficients. The maximum yield here refers to the maximum potential yield without management constraint. The crop maximum uptake rates are derived from local crop plateau yields under ideal conditions, or derived from successful crop growth models (e.g., CERES-Maize for corn). Therefore, the actual crop yield associated with N uptake in N-SIMULATOR varies with changes of environmental factors and management practices. However, the actual yields will not exceed the maximum potential yields in the model but could exceed the maximum recorded yields in the region. In other words, N-SIMULATOR cannot be used to predict a crop yield without knowing the maximum regional yield. In the implementation of N-SIMULATOR, the amount of N uptake is determined by the balance of plant demand N and soil N supply potential.

Plant Demand Nitrogen and Crop Development

The plant demand of nitrogen varies with the crop development stages. Nitrogen is usually taken up at a greater rate during the vegetative period of growth for many agricultural crops (Jones *et al.*, 1984; Rendig and Taylor, 1989; Black, 1993). Growth indexes such as N uptake rates (related to total biomass), rooting depths, and leaf area indexes are used to characterize crop development with time. The growth curves (growth indexes versus cropping days) can be used to simulate dynamics of crop N uptake and water movement (See section 4-3.3) in soil-plant systems. The uptake curves are also referred to as nutrient-absorption curves (Black, 1993). N-SIMULATOR applies the curves of N-uptake rate and rooting depth during a cropping season to estimate N absorbed by crops (Fig. 4-2.5). The curves are useful for dynamically tracing crop N uptake in simulating crops that have stable biological characteristics in local conditions. There are three methods to obtain N-uptake and rooting curves for a crop: (1) Observation in local experiments or fields. This is the preferred method. (2) Extract from literature or modeling results (Jones *et al.*, 1991a). This method works well in many cases (Ling, 1996) if the simulated crops have local data to describe the curves. (3) Use a normalized (or hypothetical) curve as default

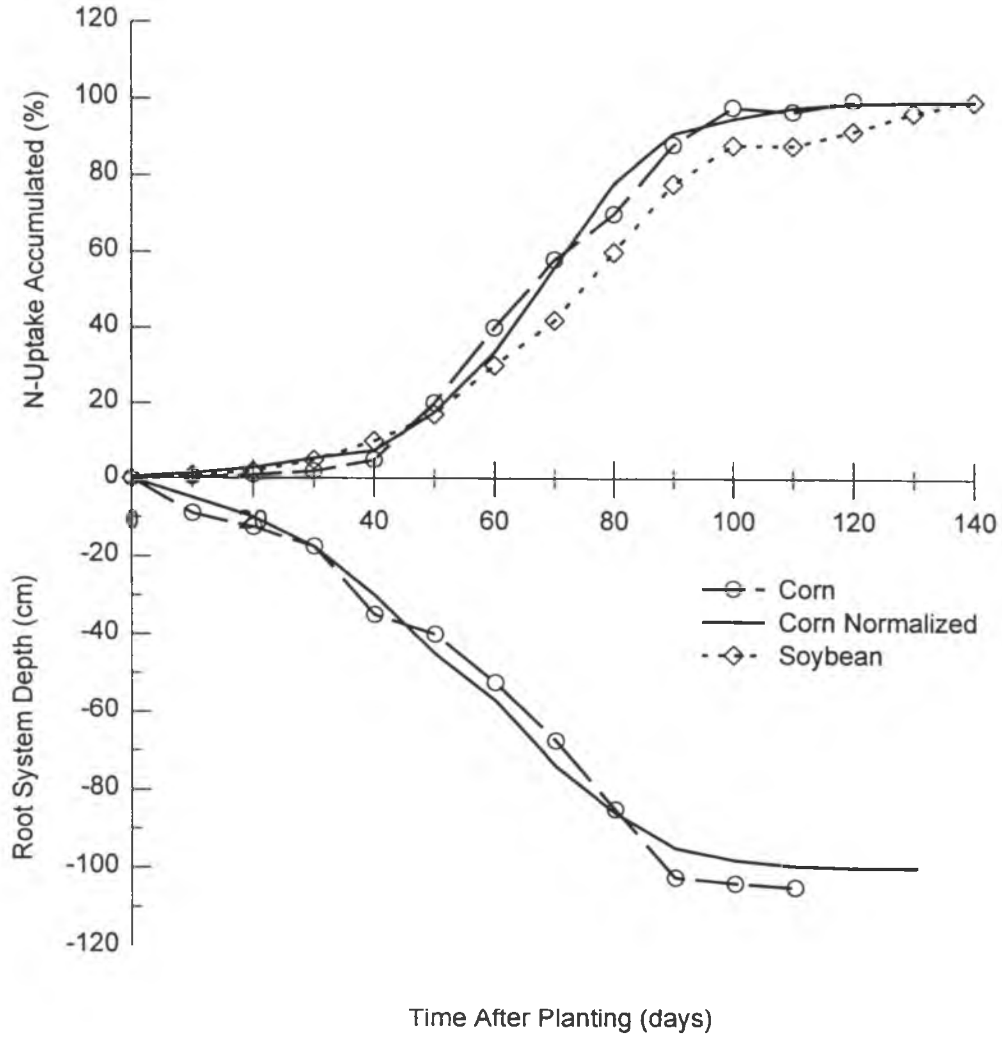

Fig. 4-2.5. Nitrogen-uptake curves represent percentage of maximum amounts of N in above-ground tissues of corn (Sayre, 1948), and soybean (Hammond et al., 1951). The corn rooting curve was simulated in Siliwa soil (Jones, et al., 1991).

(Fig. 4-2.5). NLEAP model used a normalized N-uptake curve to estimate crop nitrogen demand (Shaffer *et al.*, 1991). The advantage of this approach is that the model can be used to simulate N absorption by most plants without their genetic coefficients. Using normalized curves can produce acceptable estimates in many crops if there are no observed curves (Fig. 4-2.5).

Using the nitrogen-uptake curve, N-SIMULATOR estimates the daily plant demand for nitrogen from a daily fraction of the potential maximum N uptake rate:

$$N_{PlantDemand} = F_{Daily} \cdot N_{MaxUptake} \qquad [4\text{-}2.6]$$

where, $N_{MaxUptake}$ is total maximum potential N uptake of a crop, F_{Daily} is the daily fraction of total uptake N and can be derived from the plant nitrogen-uptake curve shown in Fig. 4-2.5.

Soil Nitrogen Supply Potential

Soil N supply potential is a measurement of the soil's capacity to provide N for a crop. In the implementation of N-SIMULATOR, soil N supply potential is used to estimate how much N a crop can absorb from soil at a certain concentration of soil inorganic N. Like the rate of plant nutrient absorption, soil N supply potential is a function of concentration of soil inorganic nitrogen (NH_4 and NO_3) and the capacity of plant uptake. The relationship between plant nutrient absorption rate and nutrient concentration supplied is often described by the curve of the Michaelis-Menten kinetic equation (Rendig and Taylor, 1989). The CERES-N model uses exponential equations to describe availabilities of inorganic N for crops (Godwin and Jones, 1991). In the common range of field concentration of inorganic nitrogen (Cahn *et al.*, 1992), this exponential curve may fit a portion of the curve of Michaelis-Menten kinetic equation (Fig. 4-2.6). This idea has been drawn from CERES-N to express soil N supply potential in N-SIMULATOR:

$$N_{supply} = NH_{4Supply} + NO_{3Supply} \qquad [4\text{-}2.7]$$

$$NH_{4Supply} = N_{NH4} \cdot (1 - e^{-kC'}) \qquad [4\text{-}2.8a]$$

$$NO_{3Supply} = N_{NO3} \cdot (1 - e^{-kC'}) \qquad [4\text{-}2.8b]$$

where, N_{supply} *(kgN ha⁻¹)* is soil N supply potential, a sum of ammonium supply potential $NH_{4Supply}$ and nitrate supply potential $NO_{3Supply}$. N_{NH4} *(kgN ha^{-1})* is soil ammonium content. N_{NO3} *(kgN ha^{-1})* is soil nitrate content. The coefficient *k* represents the crop capacity to absorb inorganic N. The variable *C' (ppm)* is the concentration of inorganic

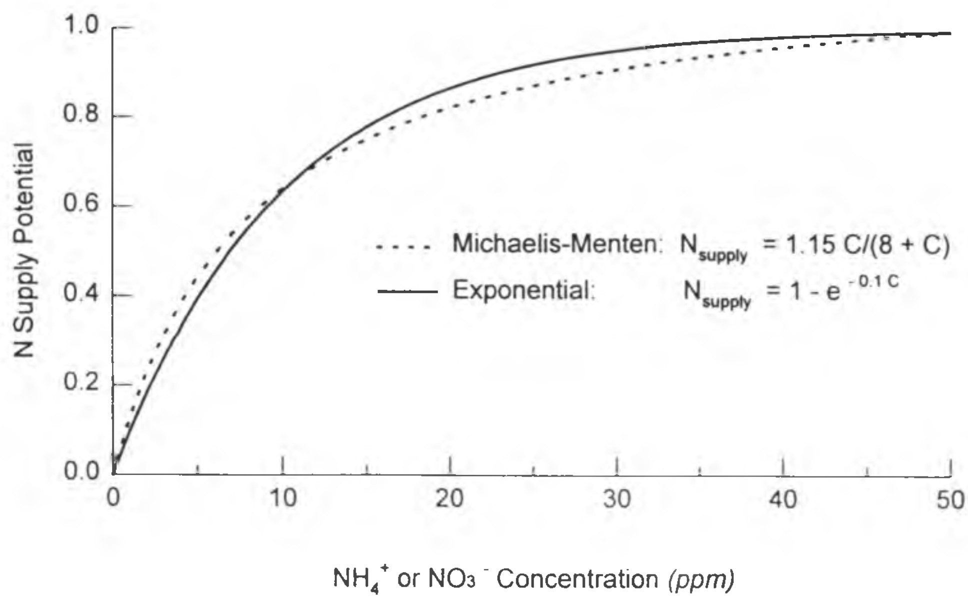

Fig. 4-2.6. Comparison of functions of inorganic nitrogen (NH_4 and NO_3) supply potential for crop uptake. Exponential function can predict N supply potential that is close to the Michaelis-Menten function prediction.

N available to the crop, which is estimated from the difference between the concentration of soil inorganic N and the minimum concentration that the crop can absorb, C_{min}. For ammonium, $C' = C_{NH4} - C_{min\_NH4}$. For nitrate, $C' = C_{NO3} - C_{min\_NO3}$. Equations [4-2.8a] and [4-2.8b] illustrate that soil N supply potential is a function of soil inorganic N concentration and crop species because the coefficient k is associated with plant variety.

Nitrogen Uptake by Plants

After plant N demand and soil N supply potential are determined, N-SIMULATOR calculates the ratio of soil N supply potential to the plant demand N $Ratio_{SupplyDemand}$:

$$Ratio_{SupplyDemand} = N_{supply} / N_{plantDemand} \qquad [4\text{-}2.9]$$

where, N_{supply} is calculated by equation [4-2.7] and $N_{plantDemand}$ is estimated from equation [4-2.6]. The $Ratio_{SupplyDemand}$ values range from 0 to 1. Finally the amount of N uptake by a plant in a simulation day, N_{Uptake}, can be estimated by

$$N_{Uptake} = \sum F_{water,\,i} \cdot F_{root,\,i} \cdot Ratio_{SupplyDemand} \cdot N_{inorg,\,i} \qquad [4\text{-}2.10]$$

where, $F_{water,\,i}$ is soil water adjustment factor in layer i (Fig. 4-2.3). $F_{root,\,i}$ is a root density fraction in the layer i on a simulation day. $N_{inorg,\,i}$ is the inorganic N content in soil layer i, which represents ammonium $(N_{inorg,\,i} = N_{NH4} - N_{min\_NH4}\ (kgN\ ha^{-1}))$ or nitrate $(N_{inorg,\,i} = N_{NO3} - N_{min\_NO3}\ (kgN\ ha^{-1}))$. Equation [4-2.10] shows that N-SIMULATOR considers the amount of N absorbed by a crop from a soil layer as a function of the root density, soil moisture and inorganic N content in the layer, and the ratio of the N supply to the N demand.

Foliar Nitrogen Uptake

In addition to plant roots, leaves can adsorb N that is sprayed on their surface. N-SIMULATOR reserves an independent pool outside a plant surface to store N from foliar fertilization. The daily N adsorbed by plant leaves from this pool, N_{Foliar} *(kgN ha^{-1})*, is estimated by

$$N_{Foliar} = FLI \cdot K_{Foliar\%} \cdot N_{fert} / Days_{FoliarAdsorb} \qquad [4\text{-}2.11a]$$

where $K_{Foliar\%}$ is maximum percentage of N fertilizer that leaves can adsorb from a total N fertilizer sprayed in one application. N_{fert} *(kgN ha^{-1})* is the total N fertilizer sprayed in an application. $Days_{FoliarAdsorb}$ is number of days that plant leaves can adsorb all N remaining on their surface. *FLI* is the fraction of light intercepted by a plant. N-SIMULATOR uses this fraction to estimate a fraction of sprayed fertilizer that plant leaves can capture, assuming that both fractions have a linear relationship. *FLI* is calculated by (Zhang, 1992)

$$FLI = 1 - e^{-k \cdot LAI} \qquad [4\text{-}2.11b]$$

where *LAI* is a leaf area index. *k* is light extinction coefficient. Fleisch (1988) reported a *k* of 0.56 for a pineapple canopy. With the regression of three pineapple plantings, Zhang (1992) reported a *k* of 0.58-0.59. A *k* of 0.59 will be used to simulate a pineapple dataset from Hawaii (See section 4-5.5).

4-3. Water Movement Modules

Nitrogen solutes (NH_4^+, NO_3^-, and urea in N-SIMULATOR) are highly water-soluble and mobile in soils. They move with water flux within soils. A dynamic N model must simulate soil water movement if nitrogen leaching behavior is considered. One dimension movement, in the vertical direction, is simulated in N-SIMULATOR.

4-3.1. Water Balance

The daily water balance at the soil surface is calculated in N-SIMULATOR using the following general equation (Jury *et al.*, 1991):

$$P + I - R = ET + D + \Delta W \qquad [4\text{-}3.1]$$

where, the components are precipitation P, irrigation I, runoff R, evapotranspiration ET, drainage or deep percolation D, and water storage change ΔW in the soil profile. Net water input to the system of N-SIMULATOR is the left-hand side of equation [4-3.1] on a daily basis (Refer to Fig. 4-1.2). ET is a sum of the water output from the soil surface (evaporation) and plant (transpiration). Drainage is accounted for as water output to the below-root zone. ΔW is estimated from the difference of soil water content over a day. In the water process simulation, N-SIMULATOR first checks whether precipitation and irrigation cause runoff. Second it simulates the water movement between soil layers of the soil profile. And finally it calculates the water escaping from soil due to evapotranspiration. Nitrogen solutes (NH_4^+, NO_3^-, and urea) movement will be simulated with water movement between soil layers.

4-3.2. Runoff

Precipitation and irrigation are daily inputs in N-SIMULATOR. Surface runoff in N-SIMULATOR is simply used to estimate net water input into a soil profile, not to estimate soil erosion as in the EPIC model (Williams, 1991). Therefore, daily runoff from rainfall and irrigation is calculated by SCS curve number equation (Soil Conservation Service, 1972):

$$Q = \frac{(R - 0.2 \cdot s)^2}{R + 0.8 \cdot s} \qquad [4\text{-}3.2]$$

where, Q is the daily runoff volume (mm), R is the daily rainfall (mm), and s is a retention parameter. In N-SIMULATOR R refers to the sum of daily rainfall and irrigation. The retention parameter s can be calculated from soil runoff Curve Number (CN) by SCS equation (Soil Conservation Service, 1972):

$$s = 254 \cdot (100 / CN - 1) \qquad [4\text{-}3.3]$$

Since s is also affected by soils, land use, management, and slope, the average curve number CN2 (moisture condition 2) was associated with these factors by SCS (Table 4-3.1 and Table 4-3.2). The actual curve number used in N-SIMULATOR is adjusted by soil moisture using the equations and coefficients used in the CERES model (Godwin *et al.*, 1984).

4-3.3. Infiltration and Redistribution

Infiltration refers to water entry and vertical downward movement from a soil surface (Jury *et al.*, 1991). Redistribution means the continued movement of water through a soil profile after irrigation has ceased at the soil surface (Jury *et al.*, 1991). Infiltration was one of the earliest processes that was modeled (Klute, 1952) and many investigations of soil-plant models have included this process since then (Hanks and Bowers, 1962; Hanks *et al.*, 1969; Nimah and Hanks, 1973; Hutson and Wagenet, 1991; Jones and Kiniry, 1986). The CERES-N approach for the infiltration-

Table 4-3.1. Runoff curve numbers (CN2) for hydrologic soil-cover complexes †

Land Use or Cover	Treatment or Practice	Hydrologic Condition	Hydraulic Soil Group			
			A	B	C	D
Row crops	Straight row	Poor	72	81	88	91
	Straight row	Good	67	78	85	89
	Contoured	Poor	70	79	84	88
	Contoured	Good	65	75	82	86
	Terraced	Poor	66	74	80	82
	Terraced	Good	62	71	78	81

† For antecedent rainfall condition II, and Ia = 0.2s (Soil Conservation Service, 1972).

Table 4-3.2. Soil groups used to estimate the runoff curve number (CN2) †

Soil Group	Description
A	**Lowest Runoff Potential**. Includes sands with very little silt and clay, also deep, rapidly permeable loess.
B	**Moderately Low Runoff Potential**. Mostly sandy soils less deep than A, and loess less deep or less aggregated than A, but the group as a whole has above-average infiltration after thorough wetting.
C	**Moderately high Runoff Potential**. Comprises shallow soils ans soils containing considerable clay and colloids, though less than those of group D. The group has below-average infiltration after presaturation.
D	**Highest Runoff Potential**. Includes mostly clays of high swelling percent, but the group also includes some shallow soils with nearly impermeable sub-horizons near the surface.

† (Soil Conservation Service, 1972)

redistribution requires fewer soil hydraulic parameters than others and predicts acceptable results (Legowo, 1987). N-SIMULATOR adapted the CERES-N's methods (Jones and Kiniry, 1986) to model the infiltration-redistribution processes. The basic concepts of this approach are described here.

The amount of water that each soil layer can hold, $Water_{CanHold}$, is calculated by

$$Water_{CanHold} = Water_{Saturated} - Water_{Actual} \qquad [4\text{-}3.4]$$

where $Water_{Saturated}$ is the soil water content at saturation (*SaturatLmt*, refer to Fig. 4-2.3). $Water_{Actual}$ is the current soil water content. If the amount of water coming into a layer is less than or equal to $Water_{CanHold}$, $Water_{Actual}$ of this layer is updated by the amount of water entered. If the $Water_{Actual}$ is less than the water content at the drained upper limit (*DrainLmt*, refer to Fig. 4-2.3), no drainage occurs. Otherwise, the daily unsaturated drainage from the layer is calculated:

$$Drain_{Unsat} = K_{Drain}\,(Water_{Actual} - Water_{DrainLmt}) \qquad [4\text{-}3.5]$$

where, K_{Drain} is a drainage coefficient (unitless) for the whole-profile. Ritchie *et al.* (1989) provided a simple method to estimate this coefficient. If the amount of water coming into a layer is greater than the $Water_{CanHold}$, the water in excess of $Water_{CanHold}$ is assumed to be saturated flow and would pass to the layer below and then unsaturated flow is followed. This "gravity-drainage" is probably the major soil water movement in N-SIMULATOR for upland cropping. When soil moisture is between *PlantLmt* (the low limit of plant extractable soil water content) and *DrainLmt* (the soil water content at drained upper limit), matric-flow may occur due to the difference total soil water potential between soil layers. Differing from drainage flow, matric-flow may flow upward if the total soil water potential of an upper-layer is lower than that of the immediate lower-layer. However, this flow might have a very small influence on total water movement in a cropping season. In our preliminary simulation experiments using a procedure "*MatricPotentialFlow*" drawn from CERES-N model (Jones and Kiniry, 1986), the matric-flow was usually less than 1% of gravity-drainage. To speed the model processes, the matric-flow was not simulated in the current version of N-SIMULATOR.

4-3.4. Evapotranspiration

Since it is difficult to distinguish water vapor produced by evaporation (direct evaporation from the soil surface) and transpiration (evaporation through the plant) from vegetated lands, **Evapotranspiration** (ET), is used to describe the total process of water transfer into atmosphere from vegetated land surfaces (Rosenberg *et al.*, 1983). N-SIMULATOR uses ET to estimate the total water loss from the soil surface and the plant during a cropping season. Many models have successfully simulated ET according to a review by Molz (1981). FAO (1986) suggested a simple method, using crop coefficient K_{cr}, to estimate the evapotranspiration of a disease-free crop growth in large fields under optimum soil water and fertility conditions and achieving full production potential in the given growing environment. K_{cr} is calculated from the ratio of maximum crop evapotranspiration ET_c to potential evapotranspiration ET_p:

$$K_{cr} = ET_c / ET_p \qquad [4\text{-}3.6]$$

Potential evapotranspiration ET_p is defined as the quantity of water evaporated and transpired by a short and uniform canopy of grass for which there is no water constraint

(Penman, 1948). Although actual ET is determined by meteorological, plant, and soil factors, potential evapotranspiration is controlled by climate and varies as a function of a season. In other words, potential evapotranspiration is independent from individual water events during a cropping season (Fig. 4-3.1). Therefore, weekly or monthly potential evapotranspiration is selected as input to calculate ET in N-SIMULATOR. The Penman formula (Penman, 1948) has been widely applied by FAO in estimating potential evapotranspiration. However, the data observed from the "Class A" evaporation pan has been suggested for modeling specific local conditions (I-Pai Wu, Department of Biosystems Engineering, University of Hawaii at Manoa, personal

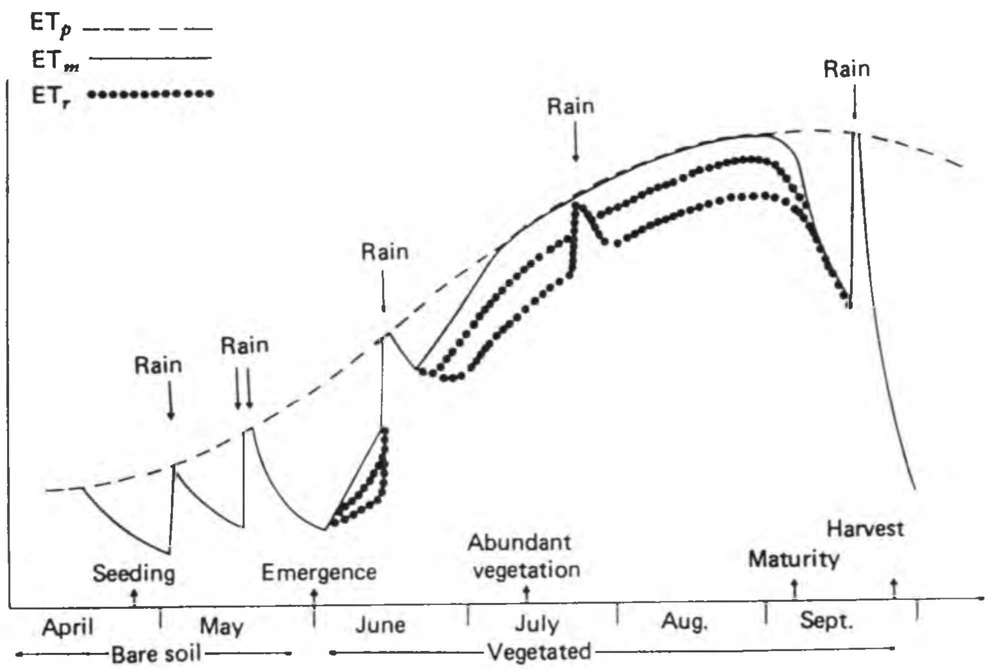

Fig. 4-3.1. The relations between potential ET_p, maximal ET_m, and actual ET_r evapotranspiration during a cropping season. Source: Rosenberg *et al.*, 1983.

communication, 1996). FAO (1986) provided a relation to estimate ET_p from "Class A" pan data:

$$ET_p = K \cdot Evaporation_{\text{"Class A" pan}} \qquad [4\text{-}3.7]$$

where K varies from 0.8 in humid tropics to 0.7 in semiarid areas, 0.55-0.65 in desert regions, and 0.9 in temperate areas with cool winters (FAO, 1986).

After the potential evapotranspiration is determined, the second step is to estimate actual ET. Crop cover is one of the most influential factors for ET. Ritchie and Burnett (1971) expressed transpiration T as a function of leaf area index LAI:

$$T = ET_p\,(-0.21 + 0.70 \cdot LAI^{0.5}) \qquad 0.1 \le LAI \le 2.7 \qquad [4\text{-}3.8]$$

Kristensen (1974) found that the ratio of ET to ET_p was a function of leaf area index LAI and approached unity at LAI of about 3 for barley, sugar beets, and grass (Fig. 4-3.2). We employed a segment function to fit Kristensen's data to calculate ET from ET_p (Fig. 4-3.2):

$$ET_{Actual} = (K_{LAI} + K_0)\,ET_p \qquad [4\text{-}3.9]$$

where K_{LAI} is the coefficient of ET_p which also is a function of LAI as follows:

$$K_{LAI} = 0.45 \cdot LAI \qquad 0 < LAI \le 1$$

$$K_{LAI} = 0.325 + 0.125 \cdot LAI \qquad 1 < LAI \le 4$$

$$K_{LAI} = 0.85 \qquad 4 < LAI$$

K_0 is the base coefficient of ET_p when there is no vegetative cover or when LAI is equal to 0. K_0 is mainly associated with soil evaporation and its values are about 0.30 - 0.35

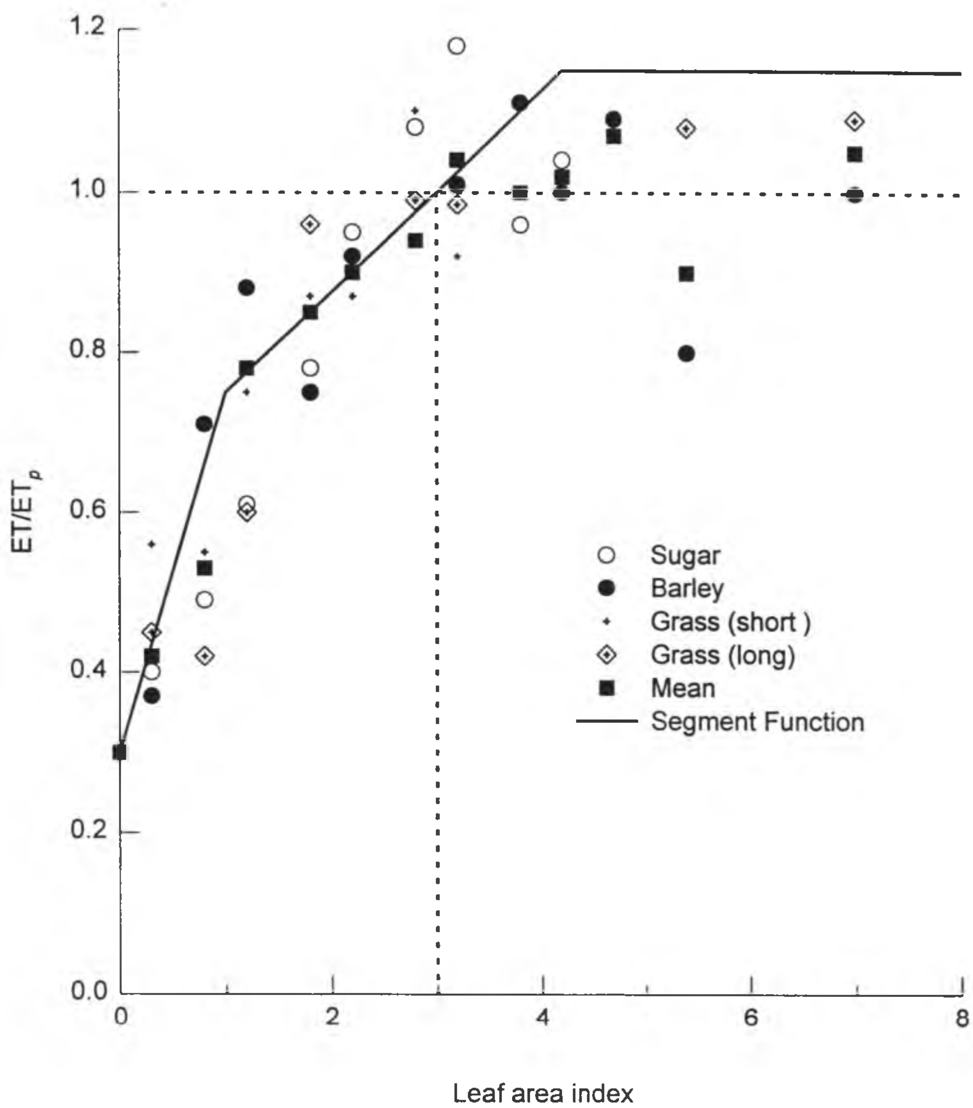

Fig. 4-3.2. Ratio of actual to potential evapotranspiration ET/ETp as a segment function of leaf area index (Redrawn from Kristensen, 1974, *Nordic Hydrology* 5:173-182).

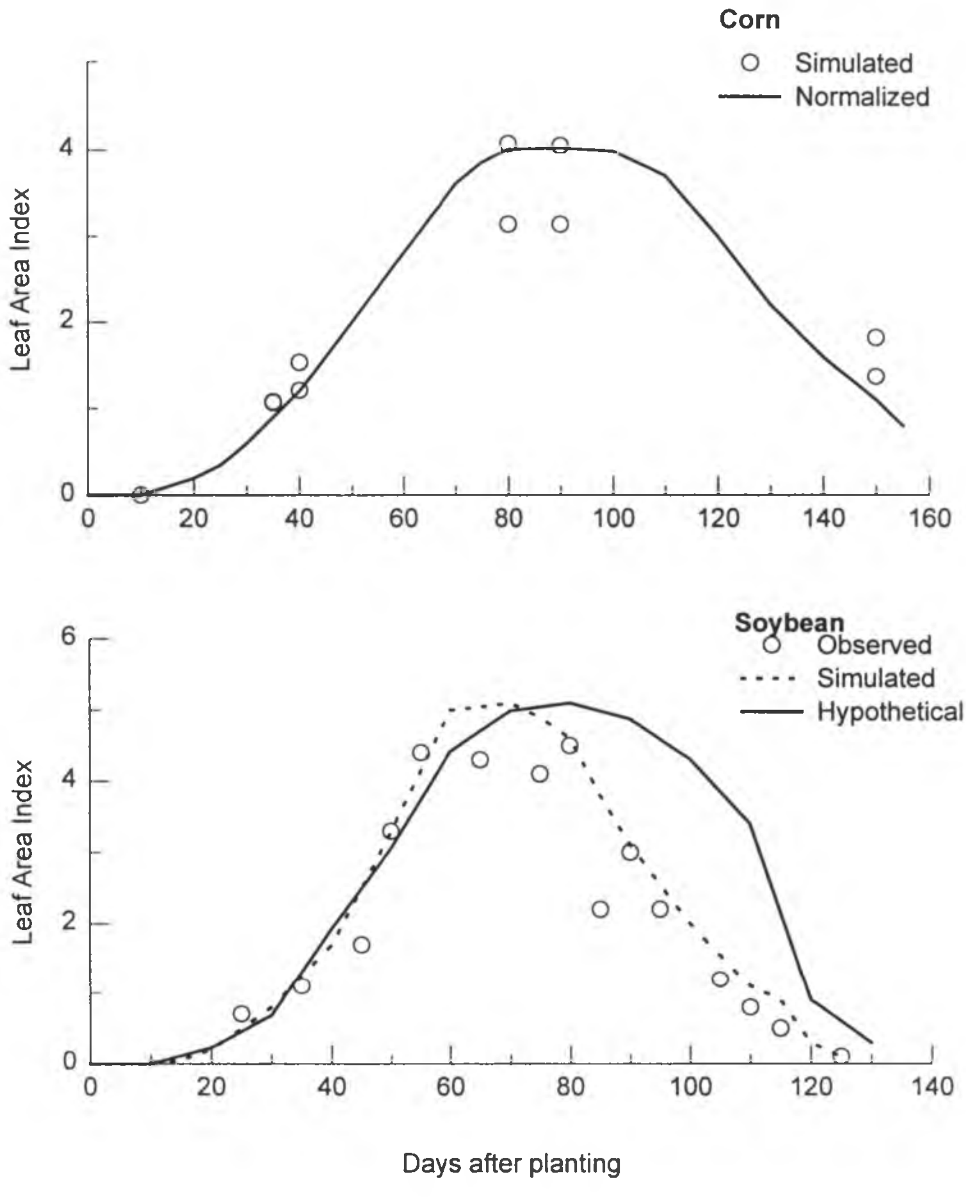

Fig. 4-3.3. Leaf Area Index as a function of plant growth stages. Sources: Corn (Bowen *et al.*, 1993), CERES-Maize simulation; Soybean (Jones *et al.*, 1984), SOYGRO simulation, Hypothetical.

in many situations (Kristensen, 1974; FAO, 1986). Fig. 4-3.3 shows examples of corn and soybean LAI-curves during a cropping season. Similar to N-uptake curves, measured LAI-curves, those cited in the literature, or normalized curves can be used in N-SIMULATOR.

Finally the soil water content decrease in a soil layer due to ET is calculated using root density distribution:

$$\Delta Water_i = - F_{rootDensity,\, i} \cdot ET_{Actual} \qquad [4\text{-}3.10]$$

where $\Delta Water_i$ is the change of soil moisture during a simulation day in the layer i, $F_{rootDensity,\, i}$ is the fraction of root density in the layer i.

4-3.5. Nitrogen Movement with Water

Nitrogen movement with soil water and across soil layers is an important process in N models associated with crop uptake and N leaching. Since NH_4^+ and NO_3^- are not electrically neutral in soil solution, their movement with soil solution may not be considered as a "free-move" as is urea. The retardation processes of ammonium and nitrate should be included in the model.

Ammonium and Nitrate Retardation

A simple linear equation is usually used to describe the chemical adsorption isotherm in soil solution systems:

$$S = K \cdot C \qquad [4\text{-}3.11]$$

where, C is the chemical concentration in the liquid phase and S is the chemical concentration in the adsorbed phase, adsorption coefficient K is the slope of the S-C linear isotherm. This linear equation can be easily inserted into other functions to model the movement of NH_4^+ and NO_3^- with soil solution. The LEACHN model (Hutson and Wagenet, 1991) consists of numerical solutions of Richards Equation for water flow in unsaturated soils and the convection-dispersion equation (CDE) for chemical transport. For an adsorbing and degrading chemical subject to plant uptake, the CDE is expressed as:

$$\frac{\partial(\theta c)}{\partial t}+\frac{\partial(\rho s)}{\partial t}=\frac{\partial}{\partial z}\{\theta D(\theta,q)\frac{\partial c}{\partial z}-qc\}-U(z,t)\pm\phi(z,t) \qquad [4\text{-}3.12]$$

where s and c are related by the sorption isotherm [4-3.11]. Ammonium adsorption was considered in many N models in temperate and tropical zones (Khan *et al.*, 1981; Hutson and Wagenet, 1991; Torbert *et al.*, 1994). CERES-N model even assumed ammonium not to be transported across soil layers (Godwin and Jones, 1991).

Bowen et al. (1993) found nitrate adsorption would greatly affect nitrate movement in a soil profile when they evaluated CERES-Maize with measured data from a series of field experiments on an Oxisol in central Brazil from 1984 through 1987. Without considering nitrate retention, CERES-Maize failed to predict the amount of inorganic N present in the soil profile and N uptake by maize (Fig. 4-3.4). To determine whether the retardation of nitrate leaching could be quantified by nitrate adsorption, they modified the model to account for a nitrate adsorption coefficient based on Wild's (1981) retardation factor:

$$V_p = 1 + K\,(\rho/\theta) \qquad [4\text{-}3.13]$$

where V_p is the number of pore volumes of water required to displace the nitrate through the soil profile, K is the adsorption coefficient, ρ = bulk density, and θ =

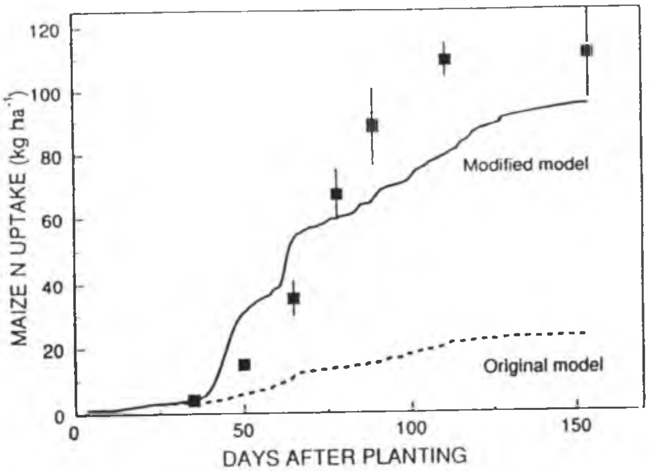

Fig. 4-3.4. Comparison of observed N uptake by maize with the CERES-Maize model prediction when accounting for nitrate retention (Modified) and not accounting for nitrate retention (Original). Source: Bowen *et. al.*, 1993.

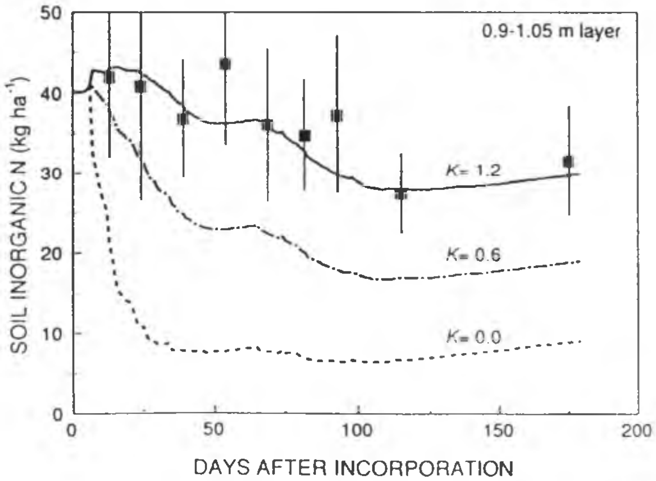

Fig. 4-3.5. Nitrate adsorption coefficient K improved CERES-Maize model in predicting inorganic N in the subsoil. Source: Bowen *et al.*, 1993.

volumetric water content. Bowen et al. supposed that the nitrate that can be moved from one layer to the next layer is only the fraction of total nitrate that is in solution *NS*:

$$NS = 1 / V_p = 1 / [1 + K (\rho/\theta)] \quad [4\text{-}3.14]$$

This modification of the model with nitrate adsorption greatly improved CERES-Maize model in predicting inorganic N in the soil profile and N uptake by the plant (Fig. 4-3.4, Fig. 4-3.5). With a resin-sand mixture as the reference system, Wong et al. (1990) measured the retardation in nitrate leaching in laboratory columns of repacked tropical soils from South America, Africa and South-East Asia (Table 4-3.3). The experimental results showed the delay of nitrate leaching as function of soil adsorption capability (an AEC measurement). A soil with delay value of 4 indicates that 4 pore volumes of

Table 4-3.3. Measured nitrate leaching retardation of tropical soils (Wong et al., 1990).

Soil	Country	Depth *cm*	pH *1:1 H_2O*	AEC *$cmol_c/kg$*	Delay *pore volume*
Alfisol	Brazil	Subsoil	5.4	0.67	5.2
Oxisol	Malaysia	35-50	5.1	1.09	4.9
Oxisol	Malaysia	20-35	4.7	0.84	4.4
Inceptisol	Colombia	40-60	5.5	1.74	4.1
Oxisol	Brazil	80-100	5.2	0.29	2.7
Oxisol	Brazil	60-80	5.0	0.22	2.3
Oxisol	Malaysia	0-20	4.3	0.20	1.8
Oxisol	Kenya	45-68	4.9	0.29	2.1
Oxisol	Brazil	80-100	4.2	0.10	1.5
Ultisol	Cameroon	40-60	5.9	0.10	1.5
Oxisol	Malaysia	35-50	4.9	0.23	1.6
Ultisol	Ivory Coast	Subsoil	4.8	0.06	1.5
Ultisol	Nigeria	47-70	4.5	0.06	1.7
Inceptisol	Colombia	60-100	6.1	0.18	1.7
Oxisol	Brazil	Subsoil	6.3	0.03	1.3
Ultisol	Thailand	80	5.7	0.01	1.0
Ultisol	Thailand	80	5.7	0.00	1.0
Ultisol	Bolivia	0-5	5.6	0.00	1.0

water were required to displace the same amount of nitrate through the soil profile than those through a soil without nitrate delay (delay value = 1). Experiments on tropical soils in Hawaii and other investigations have confirmed the retardation of nitrate leaching in acid tropical soils due to nitrate adsorption (Wetselaar, 1962; Balasubramanian *et al.*, 1973; Wong *et al.*, 1987; Deenik, 1997). Therefore, the adsorption of ammonium and nitrate are coded in N-SIMULATOR and are described below.

Nitrogen Solutes Movement Across Soil Layers

Nitrogen solutes that can move across soil layers with water flow in N-SIMULATOR are NH_4^+, NO_3^-, and urea. When a volume of water flows from a layer to the next immediate layer, the amount of the N solutes moved with water is calculated in N-SIMULATOR:

$$N_{moved} = \frac{K_d \cdot N_{total} \cdot V_{flux}}{\theta \cdot L_{layer} + |V_{flux}|} \qquad [4\text{-}3.15]$$

where, N_{moved} *(kg N · ha⁻¹)* is the amount of N solute (usually NH_4^+, NO_3^-, and urea) to be moved from a layer to the next layer. N_{total} *(kg N · ha⁻¹)* is the total amount of N solute in the layer. θ *(unitless)* is volumetric water content of the layer after V_{flux} volume of water is removed. L_{layer} *(cm)* is the thickness of the layer and V_{flux} *(cm)* refers to the volume of water to flow to the next layer (one dimension unit because of $V_{flux} = \Delta\theta \cdot L_{layer}$). ρ *(unitless)* is soil bulk density of the layer and K_d *(unitless)* is retardation factor of the N solute. K_d is calculated from the N solute adsorption coefficient K:

$$K_d = \frac{1}{1 + K \cdot \frac{\rho}{\theta + |V_{flux}/L_{layer}|}} \qquad [4\text{-}3.16]$$

In equation [4-3.15] and [4-3.16], V_{flux} is a vector because soil flow can move vertically in either a downward or an upward direction. The urea adsorption coefficient is assigned to zero. The ammonium adsorption coefficient can be estimated from soil CEC (Uehara, 1978; Uehara and Gillman, 1980; Uehara and Gavin, 1981). The nitrate adsorption coefficient can be estimated from soil AEC or soil delta pH and other soil properties (Uehara, 1978; Uehara and Gillman, 1980; Uehara and Gavin, 1981; Wong *et al.*, 1990; Deenik, 1997). The N solutes that migrate into the below-root zone represent the potential leaching portion because there are no crop roots there to absorb them, in assumptions of N-SIMULATOR. This portion of N solute (mostly nitrate) may not leach to the groundwater if the following crops have deeper root systems and no heavy water events occur during the cropping season. However, this topic is beyond the system boundaries of N-SIMULATOR.

4-4. Model Structure

N-SIMULATOR uses a mass balance approach to model the soil-plant systems, in which nitrogen and water are divided into various pools. Nitrogen pools include the pools of N in fertilizer, plant, atmosphere, and soil. N pools in soil are further divided into the forms of urea, ammonium, nitrate, and organic matter (fresh and humic, refer to Fig. 4-2.2). These pools are placed in different soil layers. The mass (N and water in the model) is transformed and transported between pools with time (a day is the minimum time interval) during a simulation cropping season. The total mass in the internal and external systems does not change in quantity at any time although the mass could be in various forms and in different pools. N-SIMULATOR was preliminarily designed to serve for Management-Oriented Modeling (MOM, see chapter 5) with database support. Therefore, N-SIMULATOR is called by MOM or a main program to run and ends with returning to MOM or the main program. We generally discuss the model structure here. Detailed information can be obtained in the source code in the Appendix, which were written in meaningful words. The flow chart of N-SIMULATOR major procedures is shown in Fig. 4-4.1. We briefly describe the main procedures below.

- **Initialization**

  When a running session is launched, N-SIMULATOR first reads the initial soil data of the root zone from databases. The data pertaining to each root zone include layer thickness, BD, soil water content at *PlantLmt*, *DrainLmt,* and *SaturatLmt*, actual soil water content, pH, root density, nutrient contents of ammonium, nitrate, urea, and organic carbon. Then the model runs in a daily loop which is nested in a weekly loop for a cropping season. The nested weekly loop is needed because of three considerations. 1) A weekly mass balance check will guarantee the precision of the simulation while not significantly slowing the simulation speed. 2) A week is an appropriate time

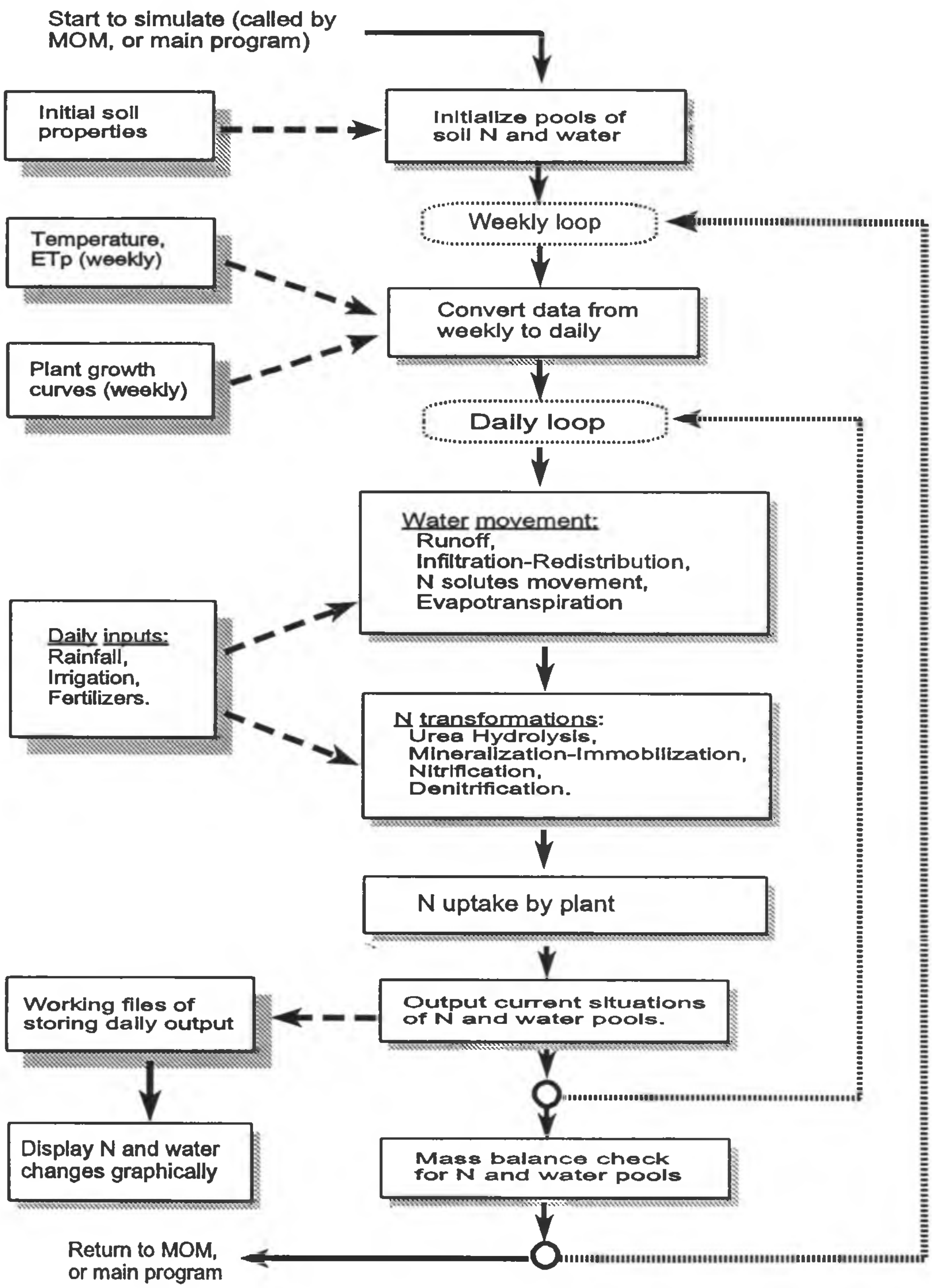

Fig. 4-4.1. Flow chart of N-SIMULATOR (major procedures)

unit for the model's work on nitrogen within-season management (See Chapter 6). 3) Weekly inputs could balance the I/O time and memory requirements.

- **Convert weekly data**

At the beginning of a week loop N-SIMULATOR first reads crop and weather data of the week which are based on daily and weekly means. The daily data of rainfall, irrigation, and fertilizer are input at the beginning of a week and are stored in temporary buffers to be used in the daily loop. This will avoid daily inputs that slow simulation while saving memory resources because of not storing the whole season data in arrays. The reason to require very fast simulation will be discussed in Management-Oriented Modeling (See Chapter 5). Weekly mean data, which include crop growth curve data (N-uptake rate, rooting depth, and leaf area index) and ET value of "Class A" pan, are converted into daily fractions to be used in daily simulation except for weekly mean air temperature. The conversion assumes that daily change rate (increase or decrease) between two weeks is linear.

- **Water processes**

Within a daily loop, N-SIMULATOR first evaluates water processes. If a daily water event (rainfall and/or irrigation) occurs, the Runoff procedure is called to calculate the amounts of runoff and infiltration. Then the amount of infiltration is passed to the Infiltration-Redistribution procedure to examine the water movement between soil layers. If N-SIMULATOR finds any water flows across soil layers, subroutine *N_MoveThroughLayers* is called to transport N solutes (ammonium, nitrate and urea) between the layers with water flows and update the N pools of ammonium, nitrate and urea. Finally Evapotranspiration procedure determines the amount of water loss due to evapotranspiration associated with the current leaf area index.

- **Nitrogen processes**

After soil water processes have been evaluated, N-SIMULATOR checks daily fertilization situations. The pools of ammonium, nitrate, urea, and organic N in top soil layer (the major root zone) are updated if the corresponding fertilizer materials are applied. Then the procedures of *Ammonia Volatilization* and *Animal Manure Decay* are executed. The above processes are assumed to occur only in the major root zone. Next, N-SIMULATOR examines the processes that occur in each soil layer. The main processes of this kind are nitrogen transformations which include *UreaHydrolysis, Mineralization-Immobilization, Nitrification*, and *Denitrification*. The N processes associated with plant growth are subsequently evaluated. *Root Distribution* procedure is called to update root densities in soil layers, and then root densities are passed to *Plant Nitrogen Uptake* procedure to estimate the amount of N-uptake in each soil layer.

- **Output and Mass balance check**

Although N-SIMULATOR has an output file called Trace.DB which is used to output any pool results for user's specific purposes, the default routines are daily outputs including pools of nitrate, ammonium, and soil water content in each soil layer, nitrate leached, N uptake by the plant, and runoff. These pools can be set to output daily or on any weekday. The outputs are saved in a working file called Simu_Out.DB and are retrieved and to be graphically displayed by the Graph procedure. The file Simu_Out.DB can be directly retrieved by Paradox for Windows or Quattro Pro for Windows (version 5.0 or higher) for other specific uses.

Before the next week's simulation begins, N-SIMULATOR checks mass (N and water) balances of this week. A week accumulated nitrogen balance error ERR_N is calculated by:

$$ERR_N\ (kgN\ ha^{-1}) = |\Delta N + N_{fert} - N_{uptake} - N_2O - N_{leach} - N_{volt}| \quad [4\text{-}4.1]$$

where ΔN is total N changes in the root zone. N_{fert} is N input from fertilizers and organic wastes. N_{uptake} is N uptake by plant. N_2O, N_{leach}, N_{volt} are N losses of denitrification, leaching, and volatilization. A week accumulated water balance error ERR_{water} is calculated by:

$$ERR_{water}\ (mm) = |\Delta W - I + ET + D| \quad [4\text{-}4.2]$$

where ΔW is total soil water content changes in the root zone. I is infiltration, ET is water loss of evapotranspiration, and D is total drainage from the root zone into the below-root zone. If the accumulated balance error, either of N or of water, is greater than 10^{-5}, N-SIMULATOR prints a warning message to the current log file.

4-5. Model Tests

The dynamic model, N-SIMULATOR, has been tested with eleven datasets from Hawaii and Brazil, to evaluate the accuracy and limitations in predicting nitrogen uptake by crops, nitrogen remaining in soil profiles, and nitrate leaching out of the root zone. The data were collected from experiments of N fertilizers and green manure in field, and an intensive and large scale field sampling in a watershed. The simulation cropping periods vary from 110 days to 400 days. The simulation soil profiles vary from 3 to 18 layers. All datasets and corresponding model parameters for the tests are available in the Appendix with electronic format on floppies and ready to run.

4-5.1. Maize, Legume Green Manure Experiment, Brazil

The dataset was described in section 2-4.1. Soil property coefficients of the dataset used in CERES-Maize were adapted to N-SIMULATOR. The crop capacity to absorb soil inorganic N (k coefficient in equation [4-2.8a] and equation [4-2.8b]) was calibrated with trial-and-error method on the control dataset. The GM treatment dataset was used to validate the model with the same model parameters.

Based on available soil data of the experiments, the soil profile was divided into six layers in depths 0 - 120 cm. The simulated total inorganic nitrogen in the root zone (0-90 cm) was compared with the observed in Fig. 4-5.1 and the simulated and the observed uptake N in maize top biomass were compared in Fig. 4-5.2. For the inorganic nitrogen contents in individual soil layers, the simulated and observed were compared in Fig. 4-5.3a and Fig. 4-5.3b. The results show that the simulated trend of nitrate changes in upper soil layers agrees with the observed while the model predicted

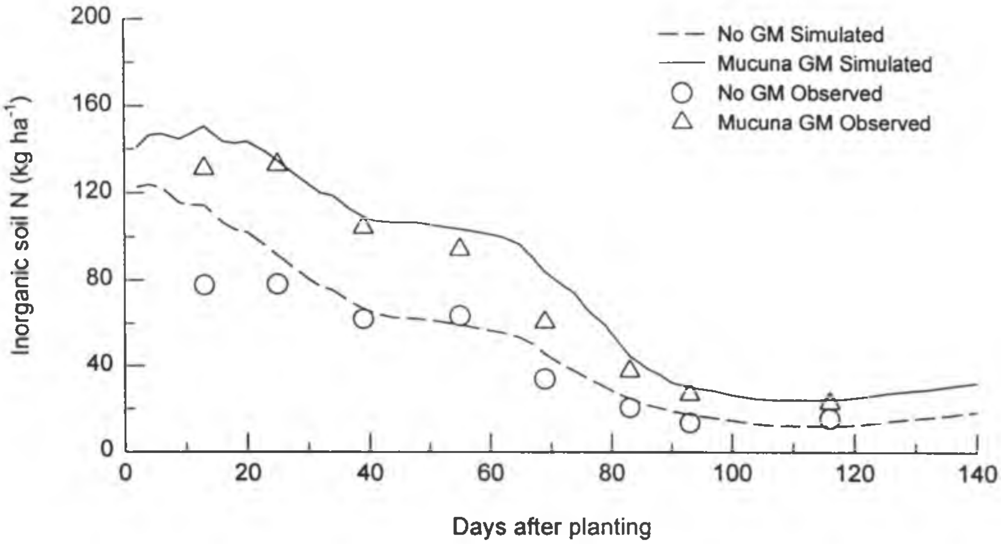

Fig. 4-5.1. N-SIMULATOR simulated and the observed total inorganic N in the soil profile (0-90 cm) of the corn fields, Brazil. Calibration for no green manure and validation for mucuna green manure.
Data Source: Bowen *et al.*, 1993.

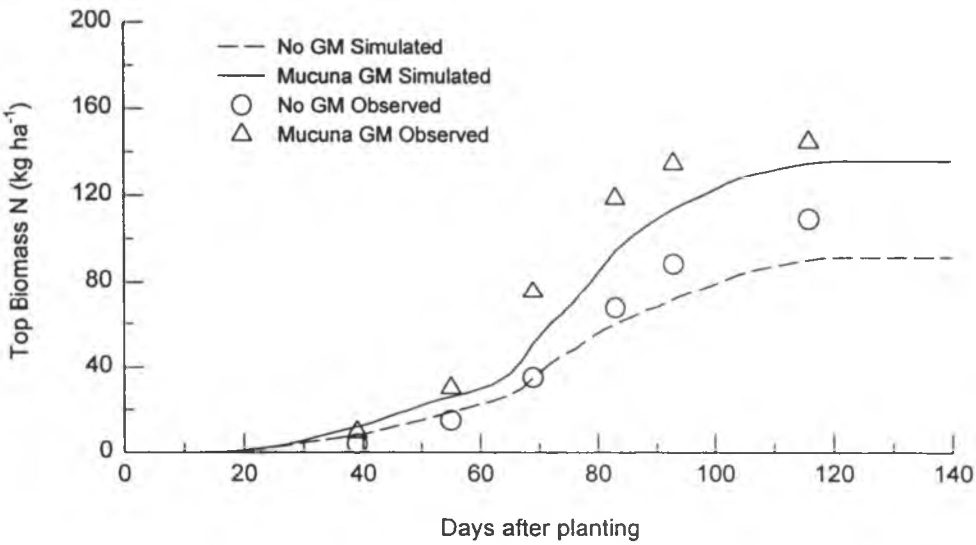

Fig. 4-5.2. N-SIMULATOR simulated and the observed corn uptake N of top biomass in the experiments, Brazil. Calibration for no green manure and validation for mucuna green manure.
Data Source: Bowen *.et al.*, 1993.

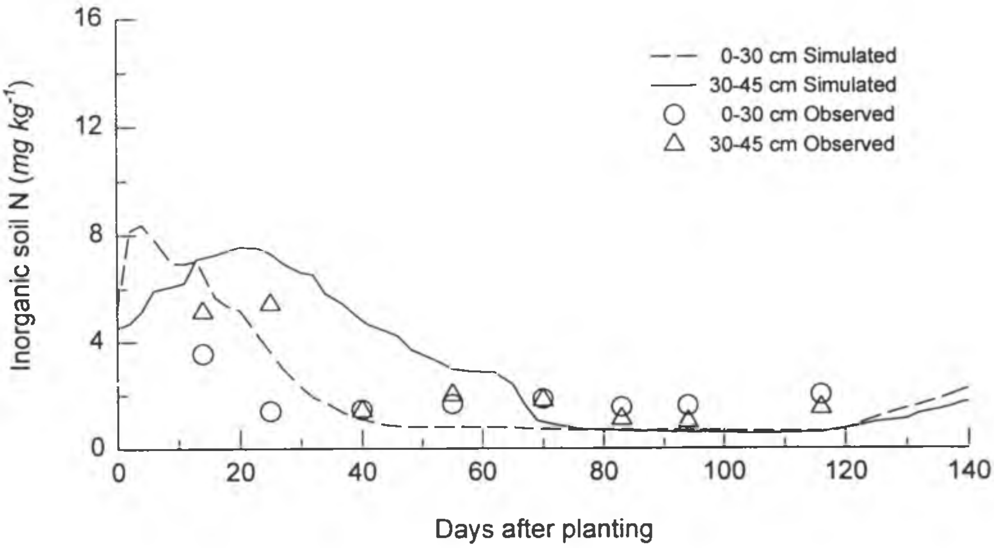

Fig. 4-5.3a. N-SIMULATOR simulated and the observed soil inorganic N in the soil profile of a corn field without green manure, Brazil. Calibration results. Data Source: Bowen *et al.*, 1993.

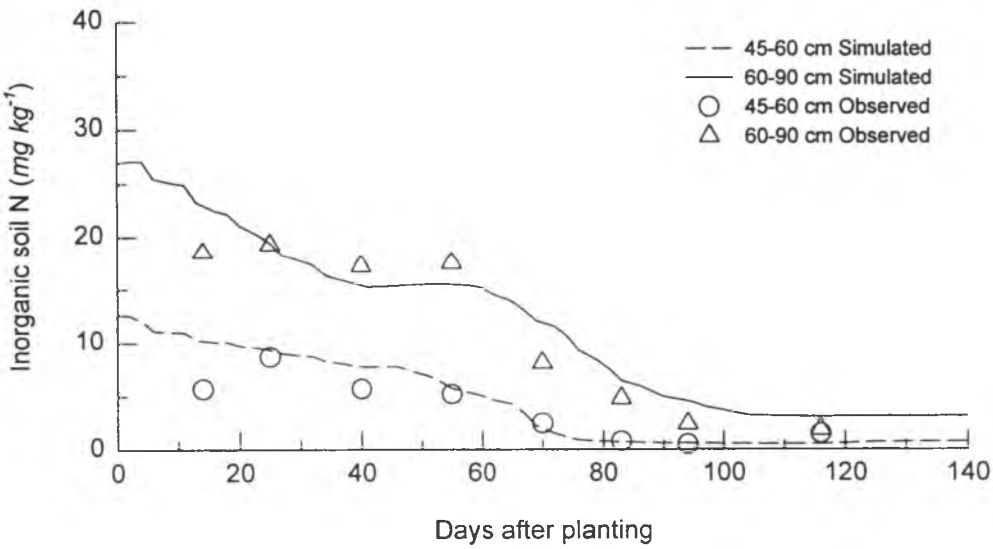

Fig. 4-5.3b. N-SIMULATOR simulated and the observed soil inorganic N in the soil profile of a corn field without green manure, Brazil. Calibration results. Data Source: Bowen *et al.*, 1993.

more precise nitrate contents in low soil layers. Predicted total inorganic nitrogen in the soil profile (Fig. 4-5.1) illustrates a better fit to the observed data than those predicted in individual layers (Fig. 4-5.3a and Fig. 4-5.3b). The 1:1 line scatter graph of the simulated and measured soil inorganic N was shown in Fig. 4-5.4a and the 1:1 line graph of the maize top biomass was shown in Fig. 4-5.4b. The model predicted slightly higher soil inorganic N than that observed while it predicted slightly lower the crop N than that observed, implying that simulated total N in the soil-crop system is quite similar to measured total N in the soil-plant system. The accuracy of the model in predicting soil inorganic nitrogen and maize uptake N of top biomass was acceptable for the purposes of the model developed in this study.

4-5.2. Maize, N Fertilizer Experiment, Hawaii

The datasets were used for validating CERES-Maize model (See section 2-4.2). Soil coefficients used for CERES-Maize were adapted to N-SIMULATOR. A trial-and-error method was employed to calibrate the maize plateau yield and the crop capacity of uptake soil inorganic N on 51 kg N ha^{-1} treatment for N-SIMULATOR. Then the coefficients and parameters were used to validate the model on 201 kg N ha^{-1} treatment.

The datasets were collected for modeling maize growth and yield and there was no soil N measured during cropping except for the initial soil condition. The nitrate content in the soil profile simulated by CERES-Maize was used to compare with that N-SIMULATOR predicted. Fig. 4-5.5a presents soil nitrate simulated by CERES-Maize during the cropping at 51 kg N ha^{-1} applied and Fig. 4-5.5b shows those

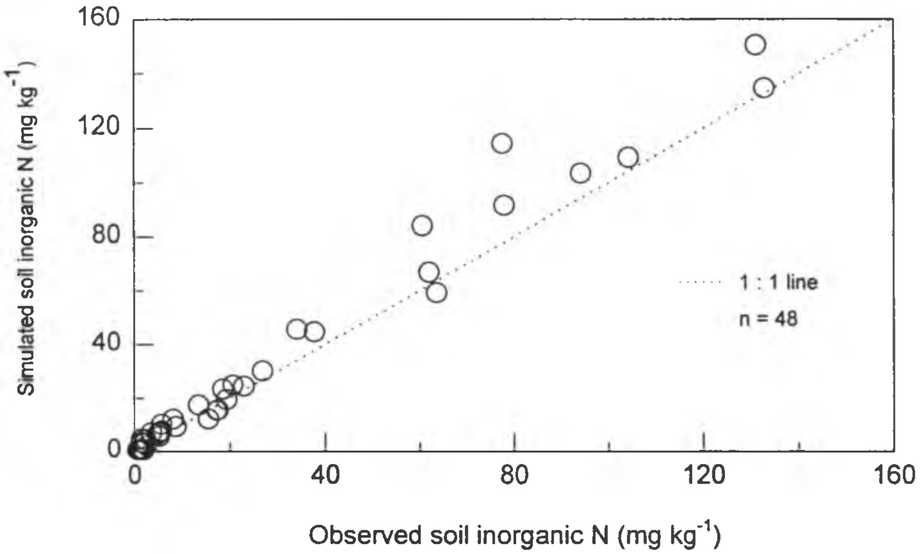

Fig. 4-5.4a. 1:1 line comparison of N-SIMULATOR simulated and the observed soil inorganic N (0-90 cm) of the corn fields with mucuna green manure or no residue, Brazil. Calibration and validation results.
Data Source: Bowen *et al.*,1993.

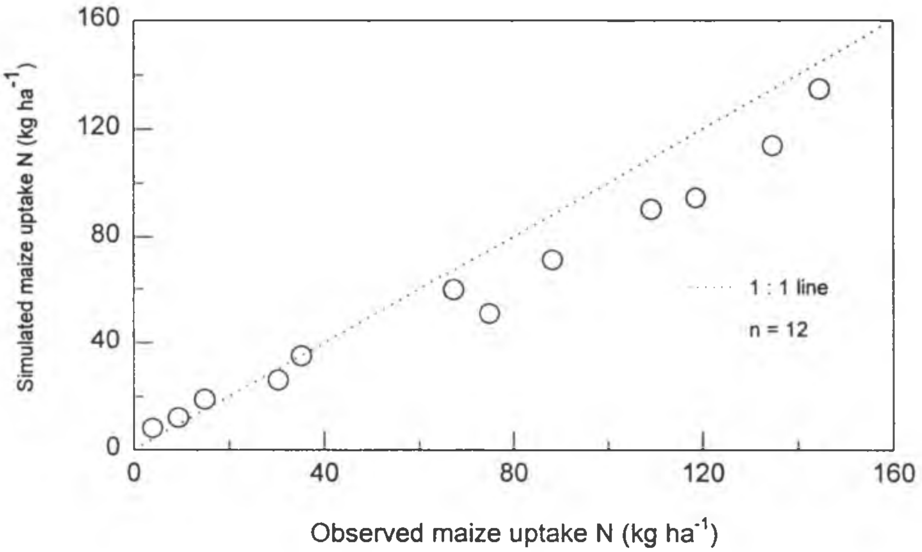

Fig. 4-5.4b. 1:1 line comparison of N-SIMULATOR simulated and the observed maize uptake N of top biomass in the experiments with mucuna green manure or no residue, Brazil. Calibration and validation results.
Data Source: Bowen *et al.*, 1993.

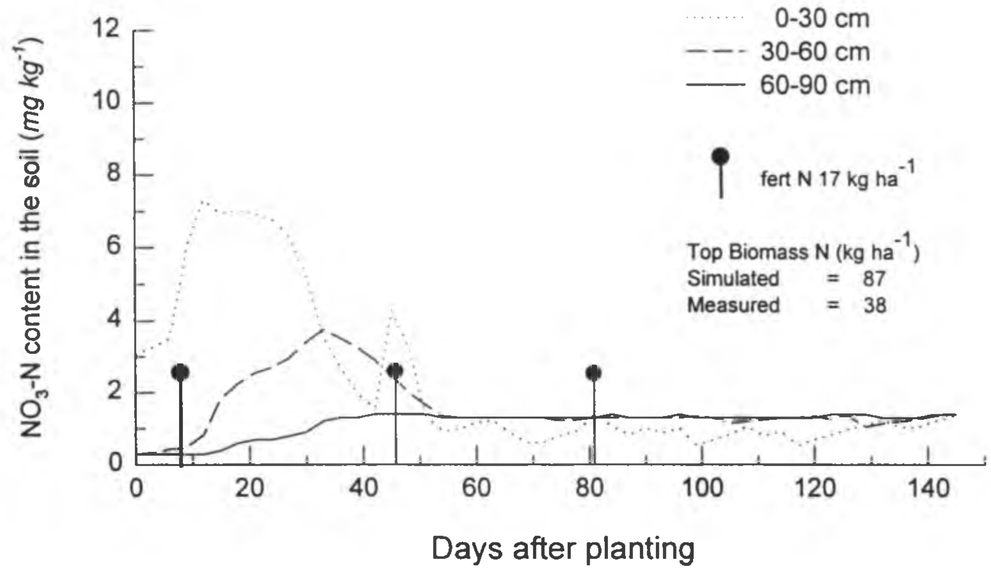

Fig. 4-5.5a. CERES-Maize simulated NO_3-N in the soil profile of a corn (X304C) field, Wahiawa soil, Hawaii. 51 kg N ha^{-1} in three applications. Data Source: Benchmark Soils Project, University of Hawaii.

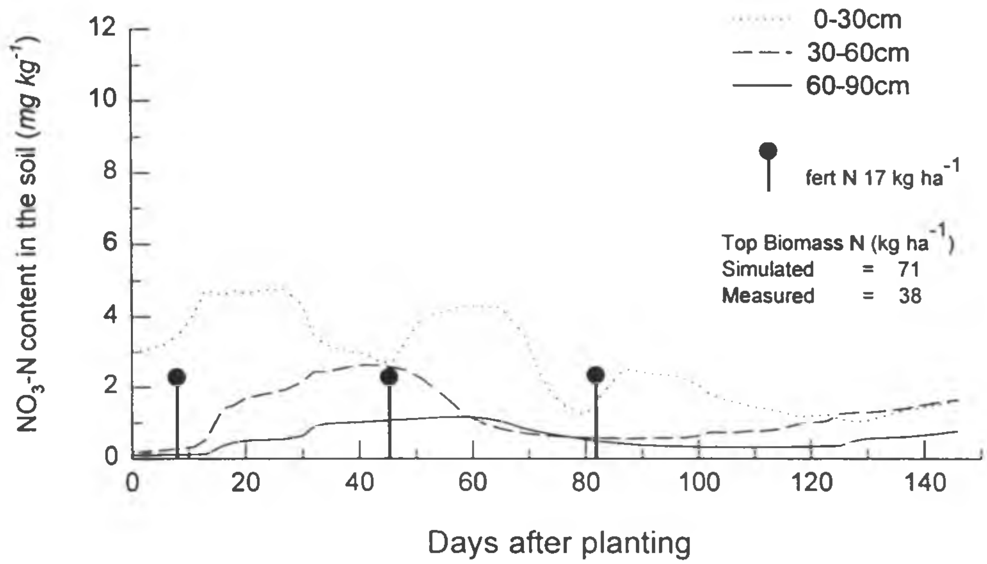

Fig. 4-5.5b. N-SIMULATOR simulated NO_3-N in the soil profile of a corn (X304C) field, Wahiawa soil, Hawaii. 51 kg N ha^{-1} in three applications. Calibration results.
Data Source: Benchmark Soils Project, University of Hawaii.

simulated by N-SIMULATOR. The N-SIMULATOR's prediction showed good agreements with the CERES-Maize's simulation in two subsoil layers (30-60, 60-90 cm). In simulating top soil layer (0-30 cm), a major root zone, N-SIMULATOR predicted more nitrate remaining in the soil than CERES-Maize predicted after second N fertilization (45 days after planting). This difference agrees with the difference of maize uptake N predicted by both models, in which CERES-Maize predicted 87 kg N ha^{-1} of maize uptake and N-SIMULATOR predicted 71 kg N ha^{-1} of maize uptake, while measured maize uptake was 38 kg N ha^{-1}. It seems that more nitrate might be remaining in the soil because N-SIMULATOR overestimated 87% of the crop uptake and CERES-Maize overestimated 129%. The similar situation occurred in simulating the 201 kg N ha^{-1} treatment (Fig. 4-5.6a, Fig. 4-5.6b). In this simulation, N-SIMULATOR overestimated 8% (or 6 kg N ha^{-1}) of the crop uptake and CERES-Maize overestimated 174% (or 127 kg N ha^{-1}). In other words, there were 127 kg ha^{-1} of fertilizer N that would have remained in soil instead of removed by the crop. The results imply that the soil nitrate content predicted by N-SIMULATOR might be closer to the real situation.

4-5.3. Maize, Field Sampling, Hawaii

Two datasets were collected from the maize fields in Hawaii (See section 2-4.3) during a winter season and a summer season.

Winter cropping season

The soil property coefficients were estimated with the procedures suggested by Ritchie *et al.* (1989). Soil nitrate adsorption coefficients were measured in preliminary

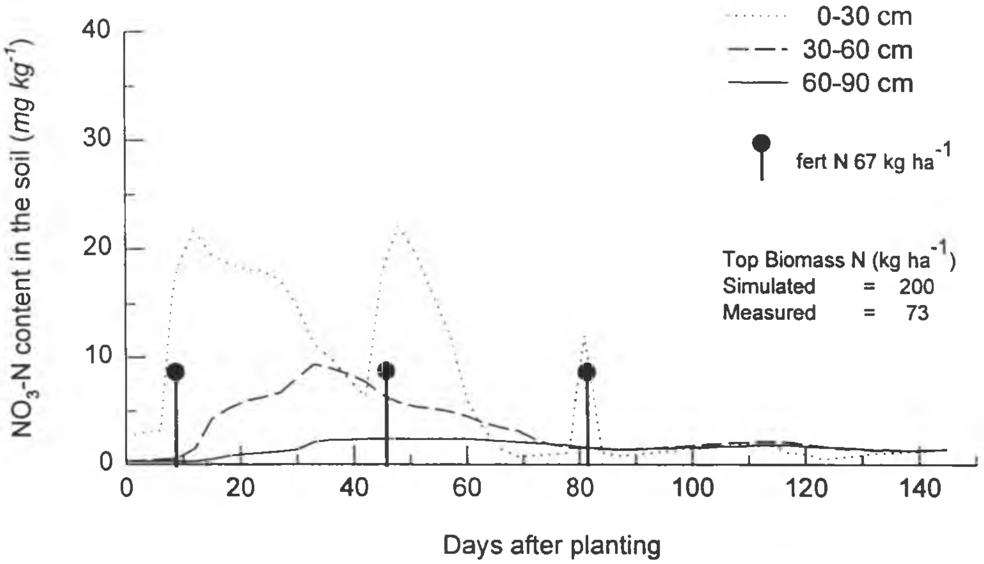

Fig. 4-5.6a. CERES-Maize simulated NO_3-N in the soil profile of a corn (X304C) field, Wahiawa soil, Hawaii. 201 kg N ha^{-1} in three applications. Data Source: Benchmark Soils Project, University of Hawaii.

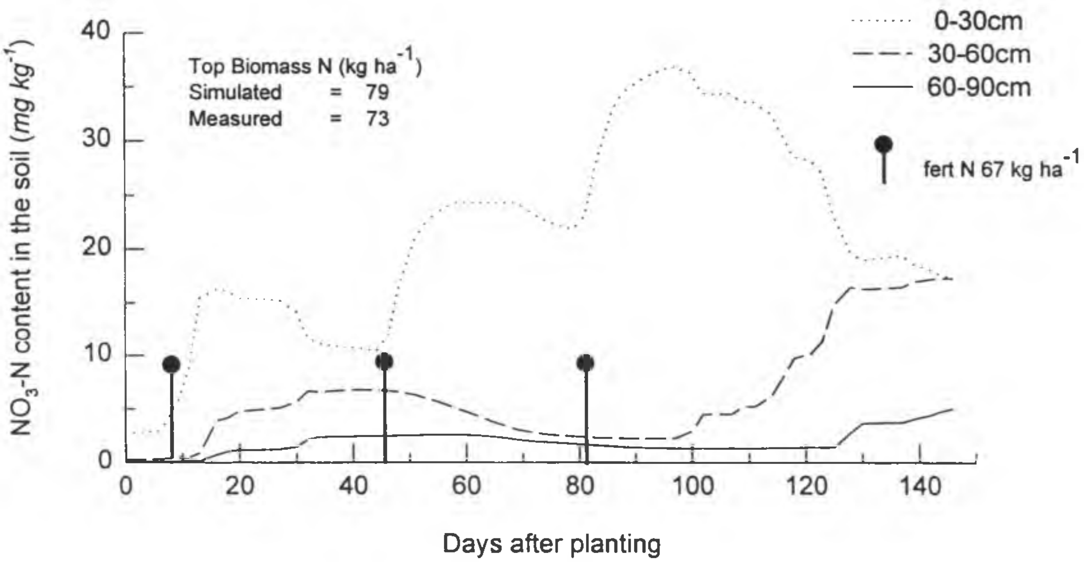

Fig. 4-5.6b. N-SIMULATOR simulated NO_3-N in the soil profile of a corn (X304C) field, Wahiawa soil, Hawaii. 201 kg N ha^{-1} in three applications. Validation results. Data Source: Benchmark Soils Project, University of Hawaii.

experiments. There were no measured crop data available. Therefore, the corn grain nitrogen content was estimated as 1.5% (Meisinger and Randall, 1991) with assumptions that straw and root contained 0.5% N, a grain to straw ratio of 1, and a straw to root ratio 6.5. The plateau yield that corn can reach was estimated as ten thousand kg ha $^{-1}$ (personal communication with Dr. Brewbaker, Department of Agronomy and Soil Science, University of Hawaii at Manoa, 1996). The crop capacity of absorbing soil inorganic N was determined using a trial-and-error method.

Fig. 4-5.7 presents nitrate content in three soil layers (the root zone and below-root zone) during the cropping. The N-SIMULATOR predicted nitrate contents agree well with the observed contents [1] except one point: observed nitrate content of 0-30 cm depth at 16-day after planting was much less than the predicted. It was not clear why the observed nitrate content at this point was so low. One fertilizer application was made 12 days before the day in which discrepancy occurred. Considering the crop could not take much nitrogen at this period of beginning growth, one possibility was an incorrect estimate of water recharge. The predicted and observed results show that nitrate content in the 30-cm of soil varies with fertilization events and crop growth while the nitrate in subsoil layers was only slightly affected (Fig. 4-5.7).

Summer cropping season

The model parameters were set the same as the winter cropping season. The plateau yield that corn can reach was estimated as 12,000 kg ha $^{-1}$ for the summer corn

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[1] The observed data is a mean calculated from $\bar{X}=10^{\frac{1}{n}\sum \log X_i}$

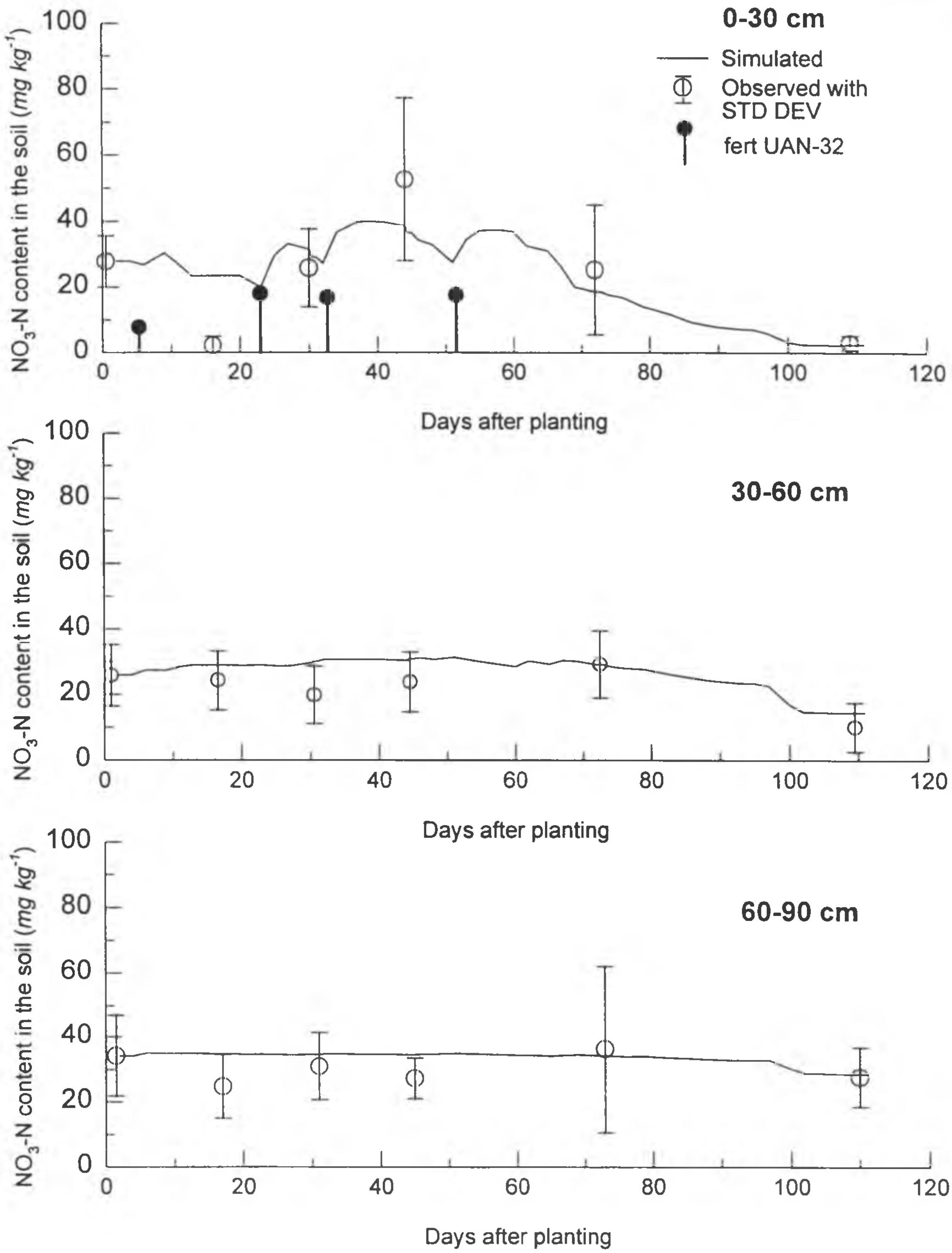

Fig. 4-5.7. Comparison of N-SIMULATOR simulated NO_3-N in the soil profile with the observed in a corn field, ICI Seeds Company, Hawaii, Nov. 1993 - Mar. 1994. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

(personal communication with Dr. Brewbaker, 1996). The nitrate content N-SIMULATOR predicted agrees well with the observed in all layers (Fig. 4-5.8). The simulated soil ammonium content in the fields was present in a low concentration (0.5 - 2.0 mg kg^{-1}) for most of the cropping days and the concentration rose only a few days after fertilizations (Fig. 4-5.9). This agrees with Khan *et al.* (1986) who measured N transformation in the Wahiawa soil (Oxisol). It also agrees relatively well with the observed data, considering that only soil samples in two sampling holes out of 12 holes were selected for ammonium analysis and ammonium in most subsoil layers was undetectable. From the aspect of modeling with time, ammonium is more difficult to simulate than nitrate in tropical uplands because it's duration in soil is much less than that of nitrate. From practical aspect, soil ammonium content in the soil was about 1-5% of nitrate and had a small influence on soil inorganic nitrogen. The simulation results for ammonium were considered acceptable.

The simulation accuracy of the model predicting soil nitrate for two cropping seasons was examined in the 1:1 line graph scattered with 30 observations (Fig. 4-5.10). Comparing Fig. 4-5.10 with Fig. 4-5.4a, the simulation accuracy for ICI maize field data was less accurate than the experiments in Brazil. It is no doubt that the simulation quality depends on the model quality and dataset quality. The data quality of a careful designed and conducted experiment is usually higher than that collected from fields. For example, soil NO_3-N (0-150 cm) in the summer maize dataset increased by about 176 kg N ha^{-1} (from 246 to 422 kg N ha^{-1}) in three weeks, based on soil analysis data during the period. This increased soil N was much higher than the

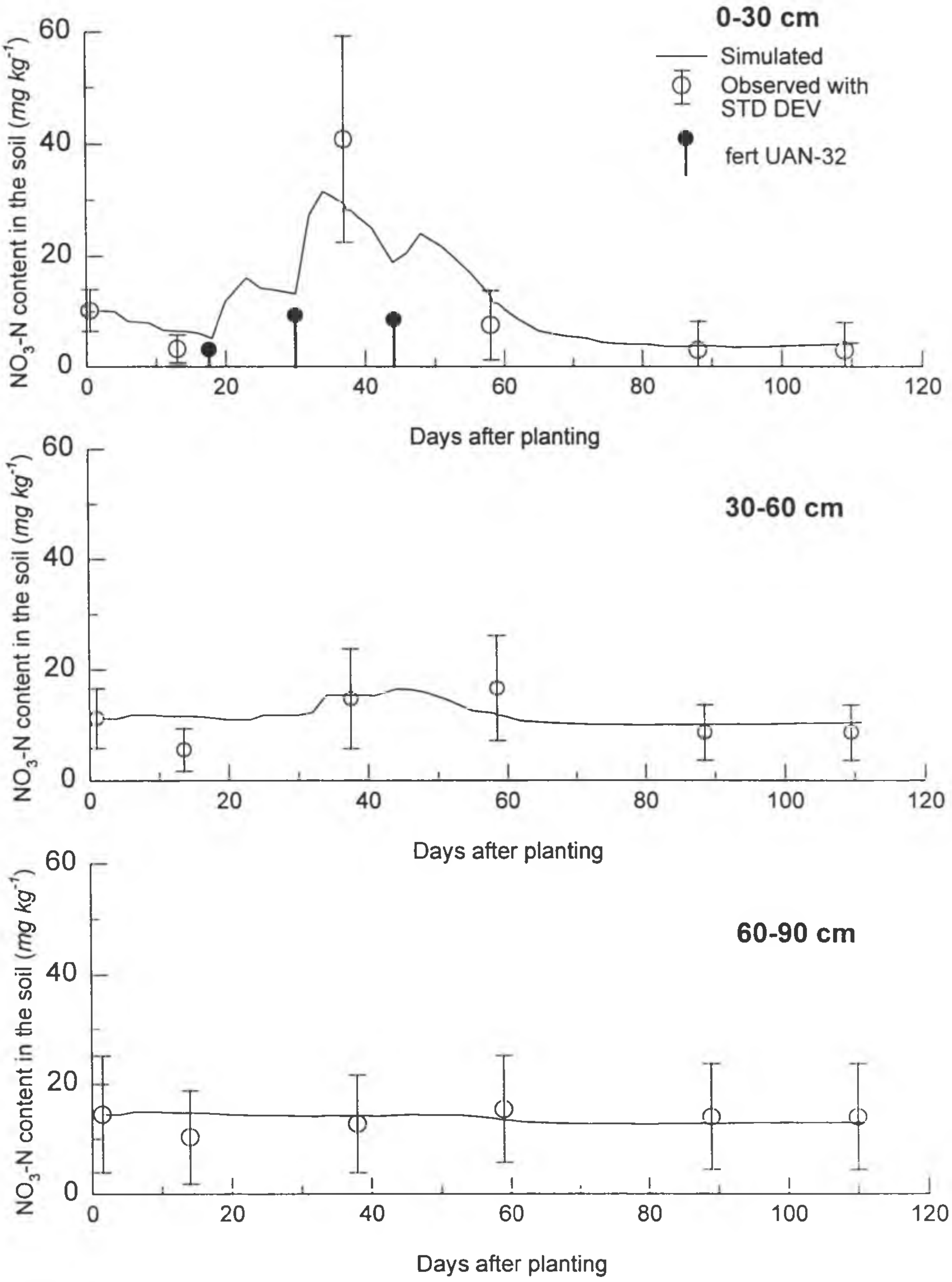

Fig. 4-5.8. Comparison of N-SIMULATOR simulated NO_3-N in the soil profile with the observed in a corn field, ICI Seeds Company, Hawaii, May-Sept. 1994. Validation results. Data Source: El-Kadi, 1996; Ling, 1996.

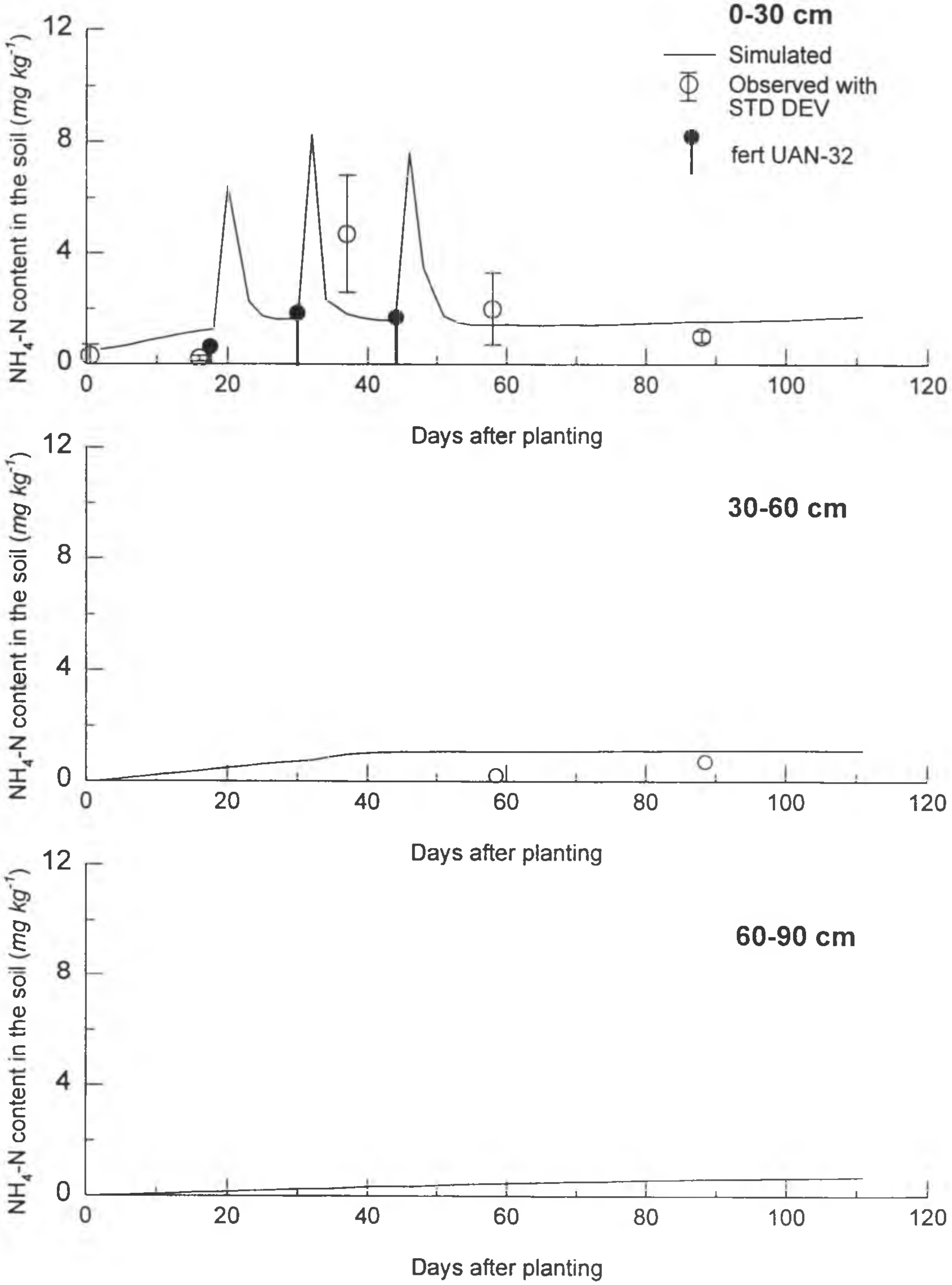

Fig. 4-5.9. Comparison of N-SIMULATOR simulated NH_4-N in the soil profile with the observed in a corn field, ICI Seeds Company, Hawaii, May-Sept., 1994. Validation results. Data Source: El-Kadi, 1996; Ling, 1996.

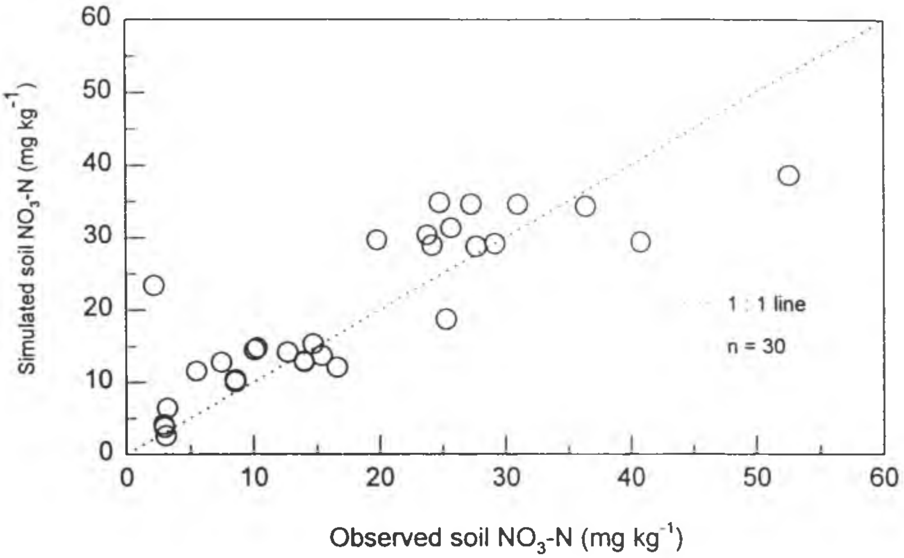

Fig. 4-5.10. 1:1 line comparison of N-SIMULATOR simulated and the observed NO_3-N in the soil profile in the corn field, ICI Seeds Company, Hawaii, 1993-1994. Calibration and validation results. Data Source: El-Kadi, 1996; Ling, 1996.

amount of N input to the soil-plant system during the period. Assuming there was no crop uptake, no leaching, and 5 kg N ha^{-1} input from mineralization of soil organic matter, it was still unclear where about extra 72 kg N ha^{-1} NO_3-N came from.

4-5.4. Sugarcane, Field Sampling, Hawaii

The dataset was described in section 2-4.4. Soil nitrate adsorption coefficients were measured in preliminary experiments. Other soil property coefficients were estimated from the dataset of Benchmark Soil Project in Waipio (See section 4-5.2), because of the same soil series (*Wahiawa series*) in the two datasets. Since there were no observed crop data, the sugarcane data were estimated from Meisinger and Randall

(1991) and Anders (1988) with assumptions of a straw to root ratio of 5. The crop capacity of absorbing soil inorganic N was determined using a trial-and-error method.

Simulated and observed nitrate contents in the soil profile were compared in Fig. 4-5.11. The simulated nitrate changes in soil layers agree with the observed data and the effects of fertilizer applications were reflected in the top soil layer (0-30 cm). Fig. 4-5.12 shows simulation accuracy of the model in predicting nitrate content in the soil profile with 1:1 line scatter graph. The simulated results were acceptable for the model objectives.

4-5.5. Pineapple, Field Sampling, Hawaii

Soil nitrate adsorption coefficients were measured using the procedure described in section 2-5. The dataset was described in section 2-4.5. Other soil property coefficients were adapted from the Waipio dataset (See section 4-5.2), because the soils in both datasets are *Wahiawa* soil located in central Oahu. A trial-and-error method was used to estimate the crop capacity of uptake soil inorganic N. Pineapple growth and N uptake data were obtained from personal communication (Dr. Duane P. Bartholomew, Department of Agronomy and Soil Science, University of Hawaii at Manoa, 1997) and literature (Stewart *et al.*, 1931; Zhang, 1992). Differing from fertilization methods used in other datasets, foliar applications of the N fertilizer were employed in this dataset. The model assumed that a maximum of 30% N fertilizer could be absorbed through pineapple leaves and the absorbing process took place in five days after fertilizer was sprayed.

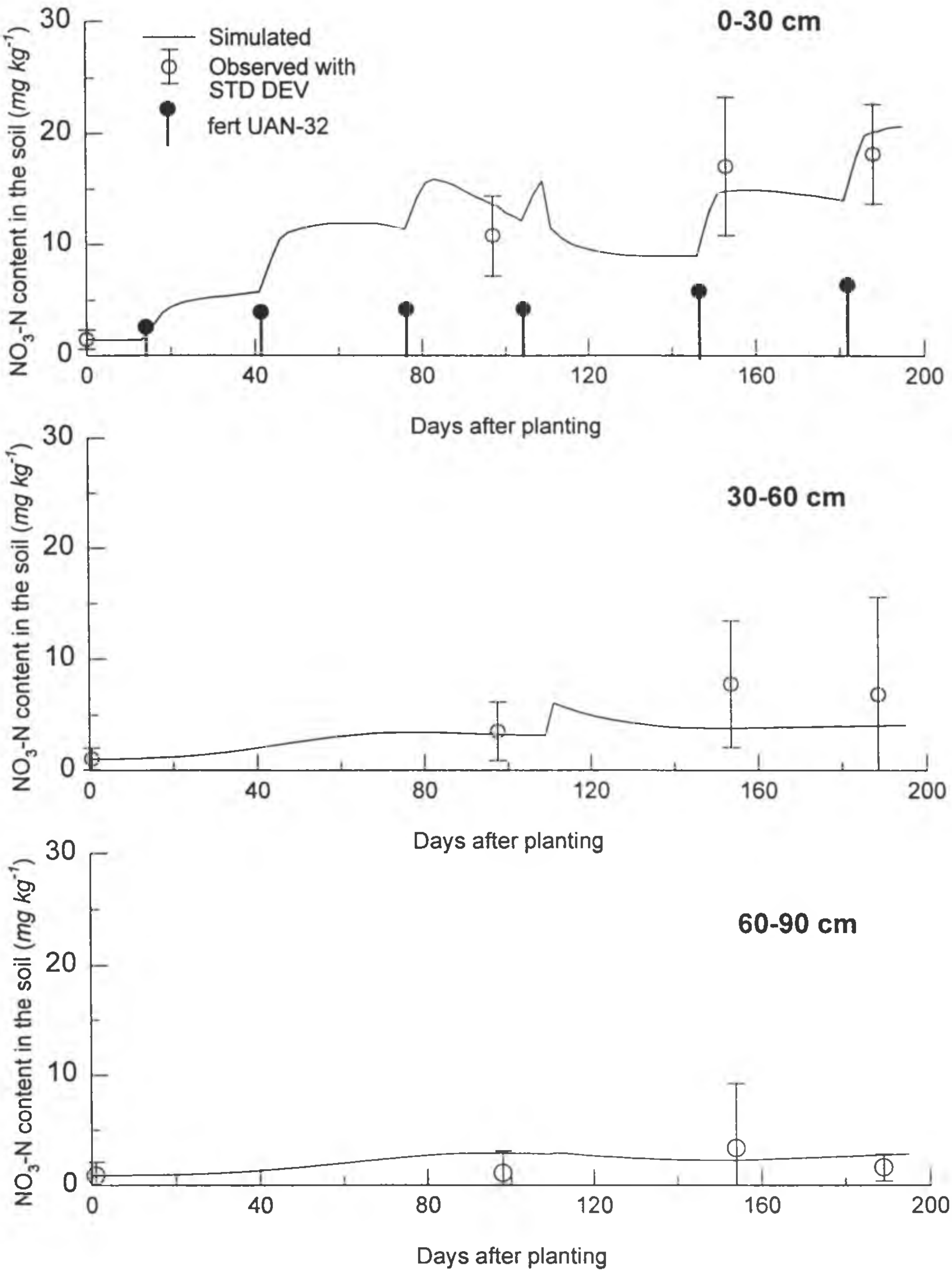

Fig. 4-5.11. Comparison of N-SIMULATOR simulated NO_3-N in the soil profile with the observed in a sugarcane field, Waialua Sugar Company, Hawaii, June-Dec., 1994. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

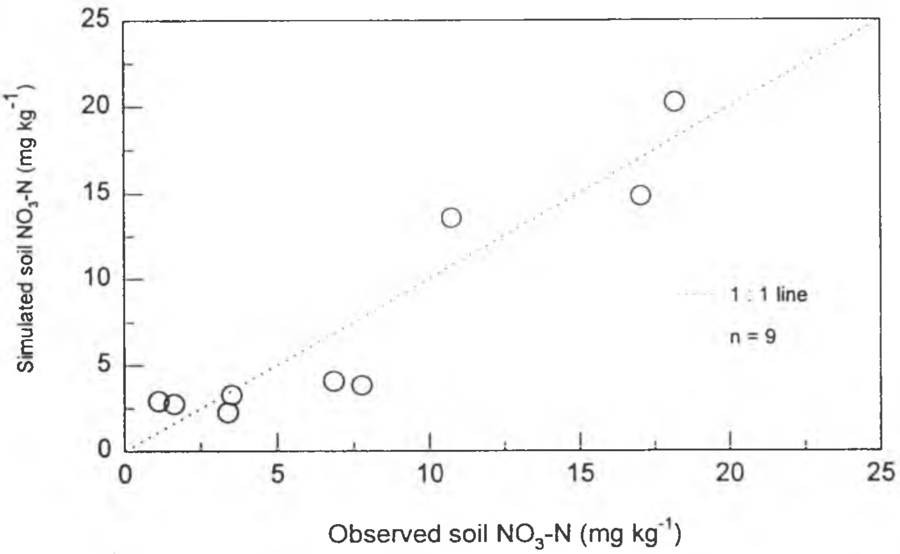

Fig. 4-5.12. 1:1 line comparison of N-SIMULATOR simulated and the observed NO_3-N in the soil profile of the sugarcane field, Waialua Sugar Company, Hawaii, June-Dec., 1994. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

N-SIMULATOR simulated and observed nitrate in the soil profile were compared in Fig. 4-5.13, Fig. 4-5.14, Fig. 4-5.15. Except for four observations in the minor root zone (30-60 cm), the simulated nitrate changes in each soil layer agree very well with the observed data over a year of crop growth. The model simulation accuracy of predicting soil nitrate was examined with 1:1 line graph (Fig. 4-5.16). For this dataset, N-SIMULATOR successfully predicted nitrate changes in the soil profile for a 400-day pineapple cropping in an Oxisol, Hawaii.

4-5.6. Nitrate Leaching, Column Experiment, Laboratory

Nitrate leaching out of a root zone predicted by N-SIMULATOR was not directly tested in any of the above datasets, although it could be tested by the nitrogen

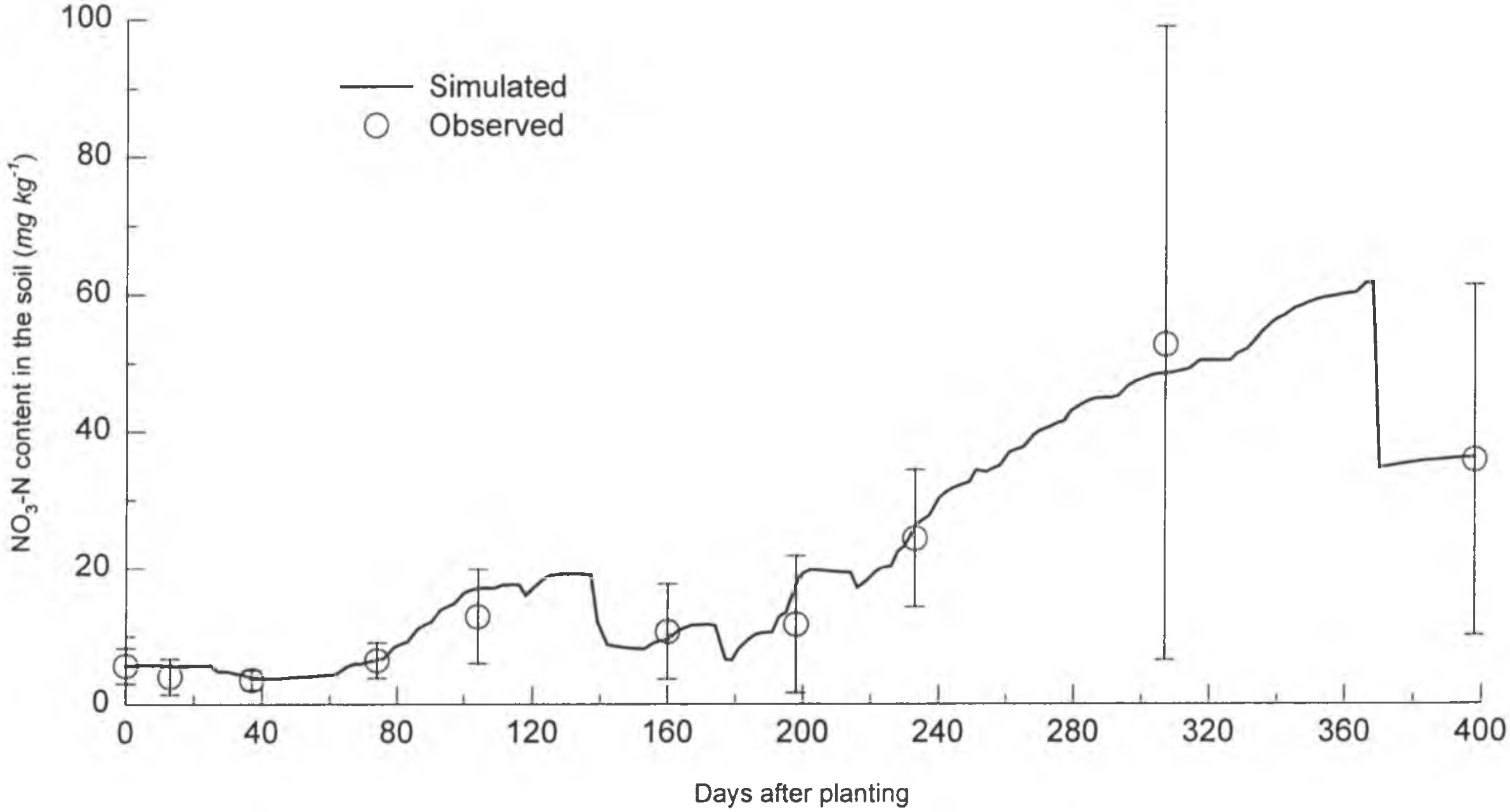

Fig. 4-5.13. Comparison of N-SIMULATOR simulated NO_3-N in the soil (0-30 cm) with the observed in a pineapple field, Del Monte Fresh Produce Inc., Hawaii, 9/30/93 -11/1/94. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

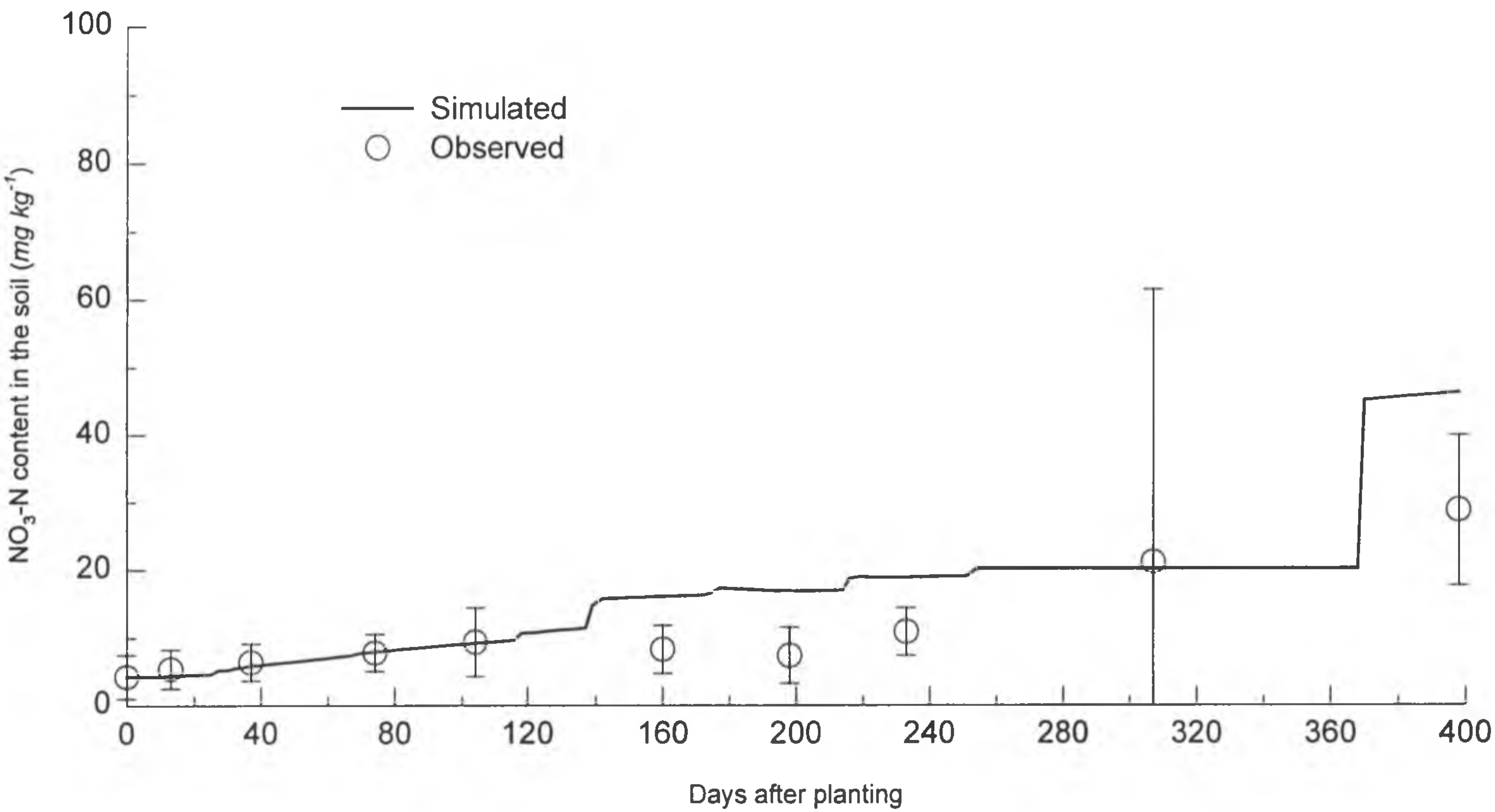

Fig. 4-5.14. Comparison of N-SIMULATOR simulated NO_3-N in the soil (30-60 cm) with the observed in a pineapple field, Del Monte Fresh Produce Inc., Hawaii, 9/30/93 -11/1/94. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

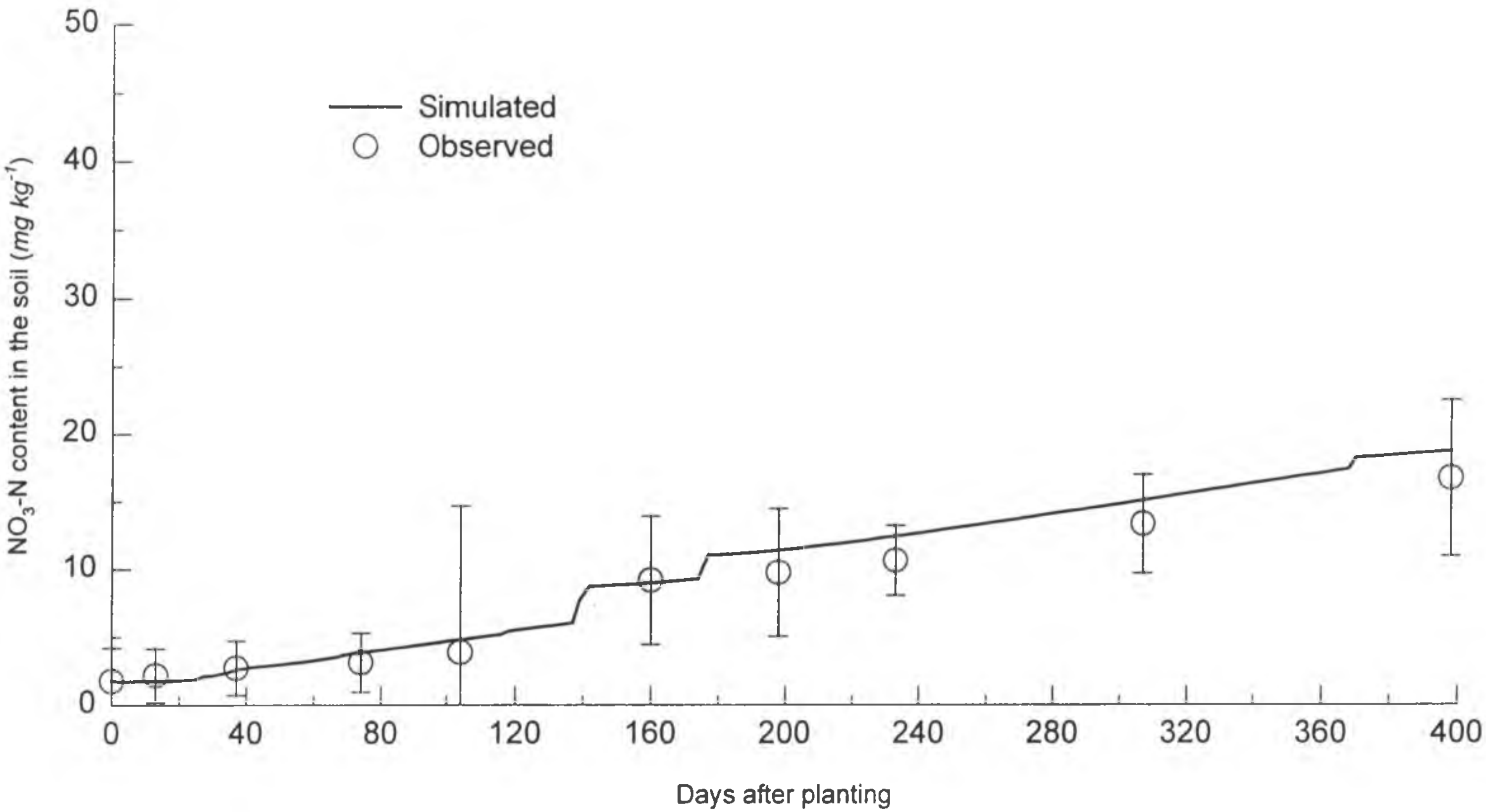

Fig. 4-5.15. Comparison of N-SIMULATOR simulated NO_3-N in the soil (60-90 cm) with the observed in a pineapple field, Del Monte Fresh Produce Inc., Hawaii, 9/30/93 -11/1/94. Calibration results. Data Source: El-Kadi, 1996; Ling, 1996.

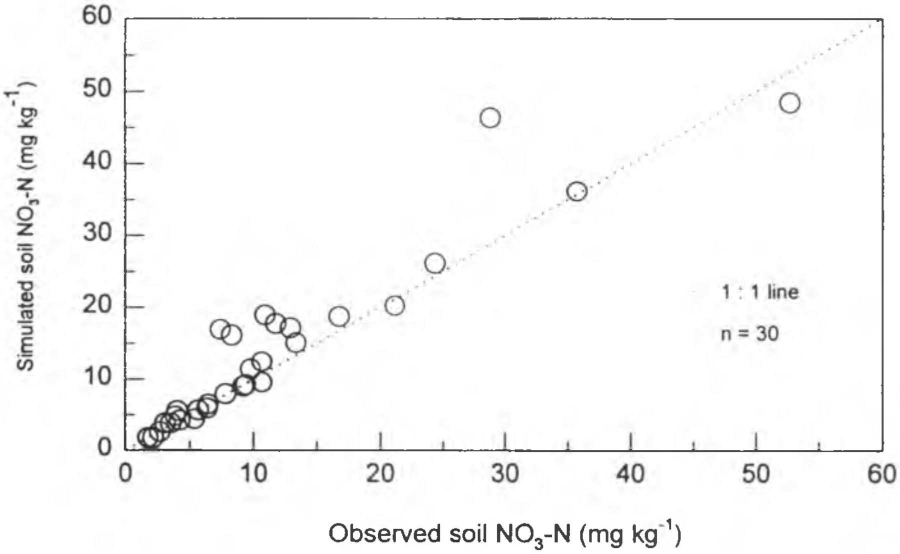

Fig. 4-5.16. 1:1 line comparison of N-SIMULATOR simulated and the observed NO_3-N in the soil profile in the pineapple field, Del Monte Fresh Produce Inc., Hawaii, 9/30/93-11/1/94. Calibration results.
Data Source: El-Kadi, 1996; Ling, 1996.

balance in soil-crop systems indirectly from the above datasets. The nitrate leaching dataset from a soil column experiment in the laboratory (See section 2-4.6) can directly test the model in predicting nitrate leaching. Liming effects on soil nitrate leaching are simulated by reducing nitrate adsorption coefficients (Deenik, 1997).

In contrast to above datasets of field experiments with cropping, this column experiment has intensive infiltration in a soil profile every day, pouring 700-900 mm 'rainfall' without crop evapotranspiration during 42-56 days. This causes soil nitrate gradients in a soil profile changed much faster than those in the field datasets. To reflect this chromatographic effect on nitrate leaching, the simulation thickness of soil layers should be as thin as possible to avoid 'diluting' (plateau) the leaching peaks.

The soil columns were divided into 18 layers (average 2.83 cm height of a layer) in the model simulations. Simulated nitrate contents in three selected layers from top, middle, and bottom of the soil profile were shown in Fig. 4-5.17a, Fig. 4-5.18a and Fig. 4-5.19a. The simulated results are expected theoretically and remaining soil nitrate contents agree with the measured data (Deenik, 1997). Simulated and observed leachate nitrate break-through curves were compared in Fig. 4-5.17b, Fig. 4-5.18b and Fig. 4-5.19b. The simulation break-through curve of the *Wahiawa* soil, with retention of nitrate leaching, shows a good fit to the observed data (Fig. 4-5.18b). Two other break-through curves also agree with the observed data but show some 'dilution' (plateau) effects. The model simulation accuracy for predicting nitrate leaching was evaluated in Fig. 4-5.20, a 1:1 line graph scattered with 80 observations. The results support the conclusion that N-SIMULATOR simulations were acceptable in predicting nitrate leaching in this laboratory soil column study.

4-6. Summary

A dynamic simulation model for the N cycle in soil-plant systems, N-SIMULATOR, was developed for Management-Oriented Modeling (See chapter 5). Major components of the model were summarized in Table 4-6.1. With the mass balance approach, N-SIMULATOR simulates nitrogen and water in a soil-plant system in diverse pools and forms. Nitrogen pools include the pools of N in fertilizer, plant, atmosphere, and soil. Soil N pools are further divided into the forms of urea, ammonium, nitrate, and fresh and humic organic matter. These pools are placed in different soil layers. Nitrogen and water are transformed and transported between pools with time during a simulation. Total mass in the internal and external systems does not change in quantity although the mass could be in various forms and in different pools. N-SIMULATOR predictions were evaluated with 11 datasets from Hawaii and Brazil. The datasets represent the situations of three crops, five locations and a laboratory experiment. Simulation cropping periods vary from 110 days to 400 days. Soil profiles were simulated from 3 to 18 layers. Calibration and validation results showed that the model simulation accuracy was acceptable in predicting N uptake by crops, inorganic N remaining in soil profiles, and nitrate leaching out of the root zone.

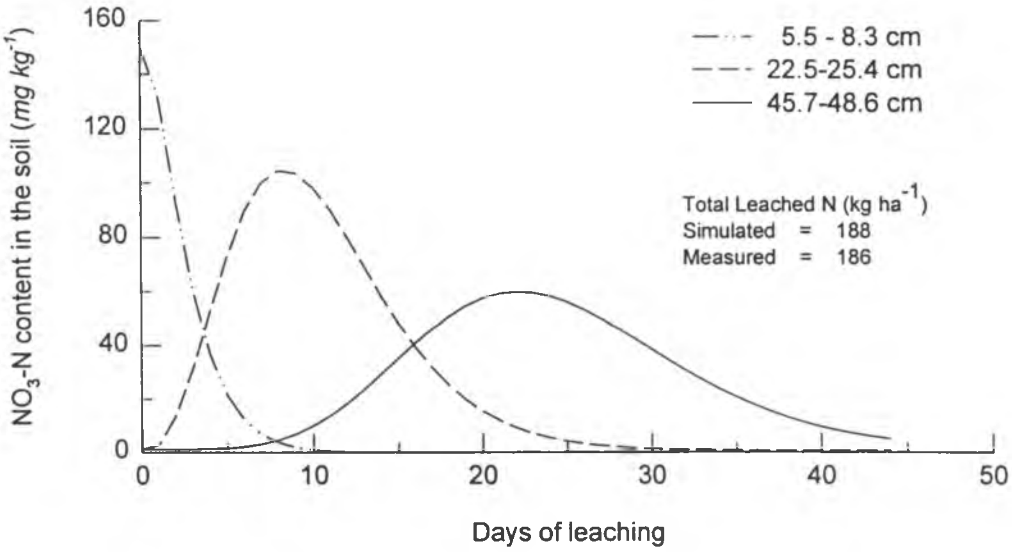

Fig. 4-5.17a. N-SIMULATOR simulated NO_3-N in the soil profile of an Ultisol (*Leilehua series*) in the leachate column experiment (flow rate 16.24 mm day^{-1}). Data Source: Deenik, Jonathan L., 1997.

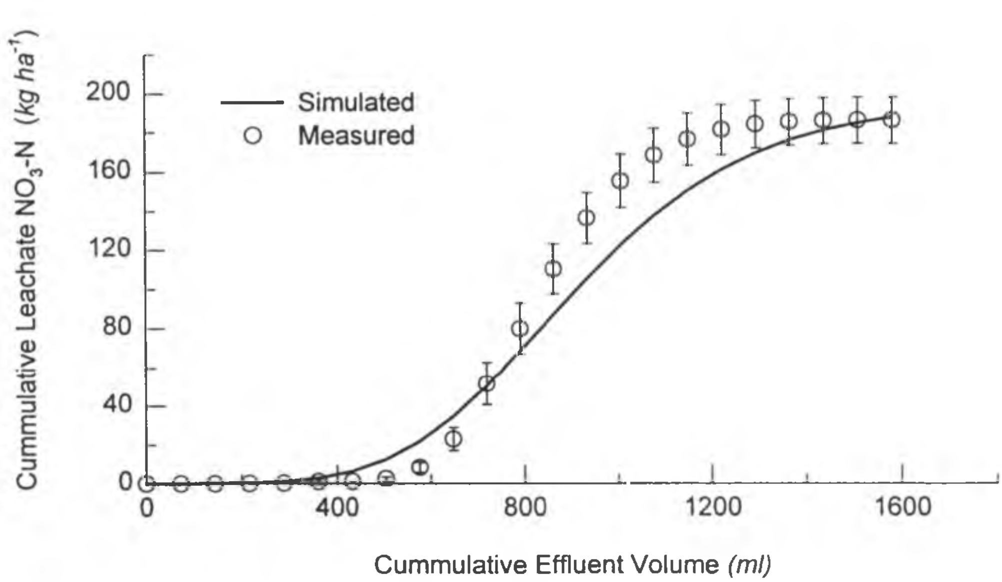

Fig. 4-5.17b. N-SIMULATOR simulated and measured nitrate break-through curve for an Ultisol (*Leilehua series*) in the leachate column experiment. Calibration results. Data Source: Deenik, Jonathan L., 1997.

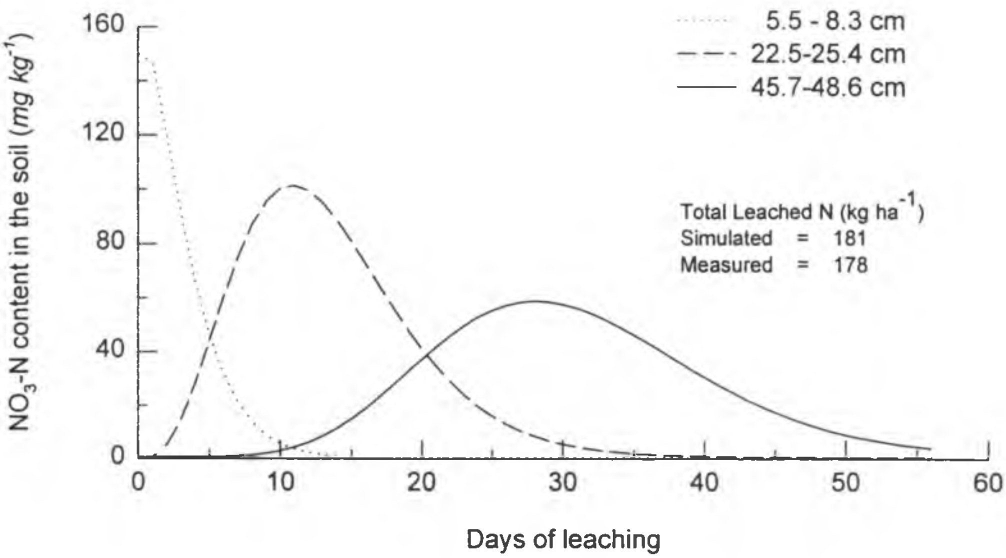

Fig. 4-5.18a. N-SIMULATOR simulated NO_3-N in the soil profile of an Oxisol (*Wahiawa series*) in the leachate column experiment (flow rate of 16.24 mm day^{-1}.) Data Source: Deenik, Jonathan L., 1997.

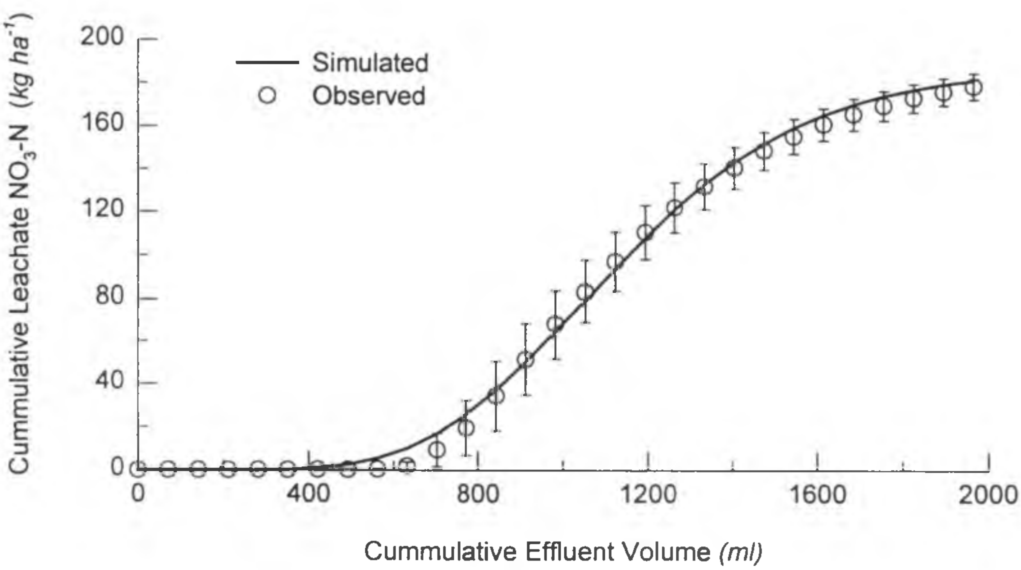

Fig. 4-5.18b. N-SIMULATOR simulated and measured nitrate break-through curve for an Oxisol (Wahiawa series) in the leachate column experiment. Calibration results. Data Source: Deenik, Jonathan L., 1997.

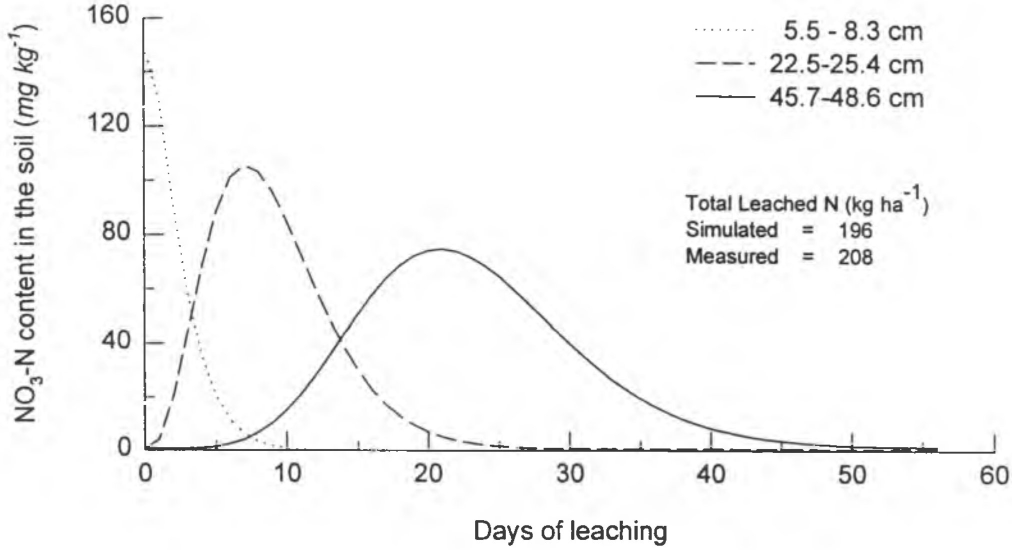

Fig. 4-5.19a. N-SIMULATOR simulated NO_3-N in the soil profile of an Oxisol (*Wahiawa series*) applied lime (4 tons ha^{-1}) in the leachate columns (flow rate 16.24 mm day^{-1}). Data Source: Deenik, Jonathan L., 1997.

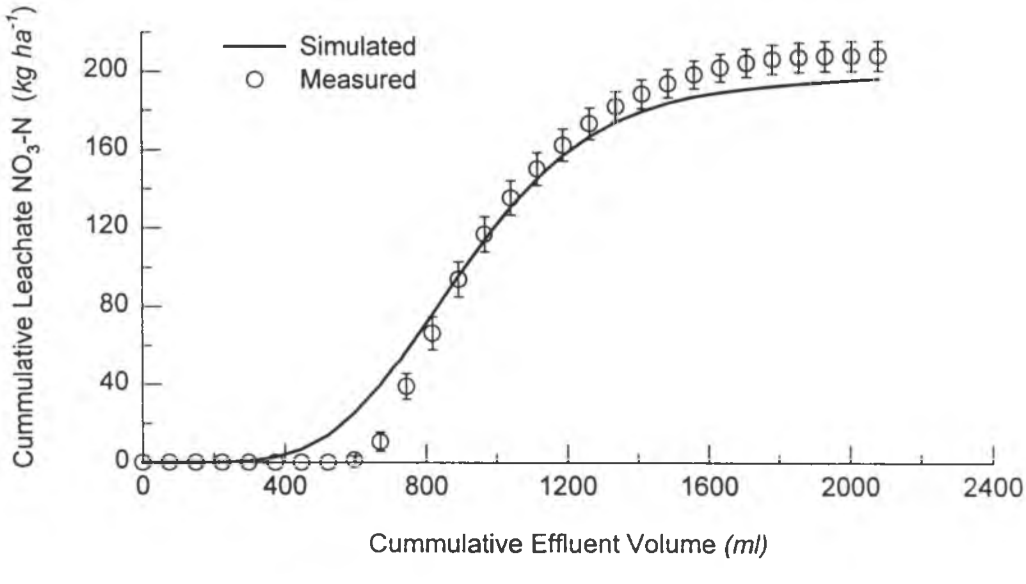

Fig. 4-5.19b. N-SIMULATOR simulated and measured nitrate break-through curve for an Oxisol (*Wahiawa series*) applied lime (4 tons ha^{-1}) in the leachate columns. Validation results.
Data Source: Deenik, Jonathan L., 1997.

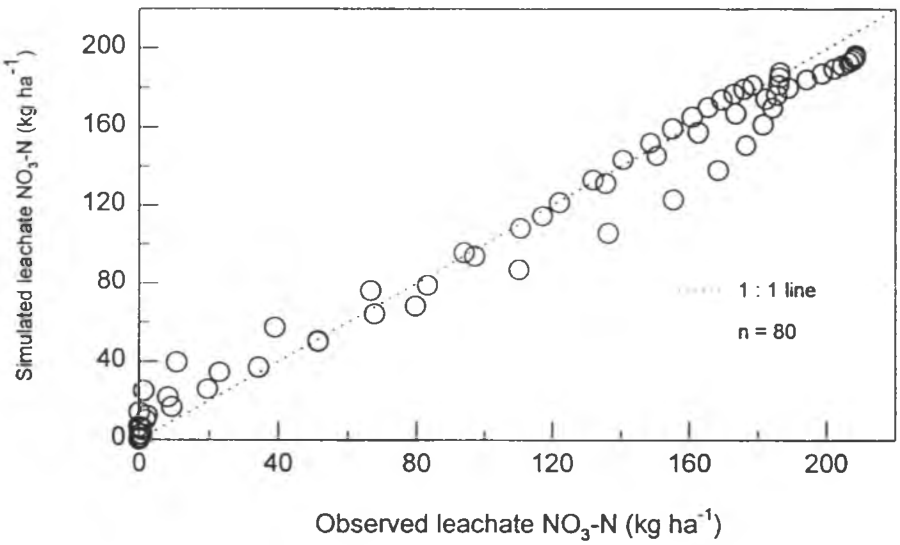

Fig. 4-5.20. 1:1 line comparison of N-SIMULATOR simulated and observed leachate nitrate in the leachate column experiment. Calibration and validation results. Data Source: Deenik, Jonathan L., 1997.

Table 4-6.1. Knowledge sources of the dynamic model, N-SIMULATOR. †

Model Component	Source	Modification
Factors of soil moisture and temperature	CERES-Maize, NLEAP, SOYGRO, Torbert '93	None
Urea hydrolysis	CERES-Maize	None
Ammonia volatilization	N-BALANCE	change Max rate from season to daily
Soil OM mineralization and Immobilization	CERES-Maize	None
Organic waste mineralization	Stanford and Smith, 1972; The authors ‡	Multiple pools and processes for various wastes
Nitrification, denitrification	CERES-Maize	Change a constant to variable
Plant demand N	NLEAP	Change rates from weekly to daily
Soil N supply potential	CERES-Maize	variable of crop uptake capacity
Soil N supply index	The authors	(See chapter 5)
Root N uptake	The authors	
Foliar N uptake	The authors	
Water balance	Jury *et al.*, 1991	None
Runoff	CERES-Maize, SCS, 1972	None
Infiltration, redistribution	CERES-Maize	No up matric-flow
Evapotranspiration	FAO, 1986; Kristensen, 1974; the authors	change ET from weekly to daily basis
Soil water supply index	The authors	(See chapter 5)
Ammonium retardation	The authors	
Nitrate retardation	Bowen *et al.*, 1993	None
N solutes movement	The authors	
Six simulation modes	The authors	(See chapter 5)

† For major components of the model.
‡ Contributions from the authors of this study (LI and Yost), based on multiple sources.

Chapter 5

Management-Oriented Modeling

There are numerous existing models that describe the nitrogen behavior under natural conditions and given management practices. Based on the inputs of soil, plant, weather and management data, these models provided predictions, evaluations, and assessments for nitrogen problems (See Chapter 3, Evaluation of Existing N Models). However, their capabilities for optimizing N management are limited. As De Willigen *et al.* (1990) state, "Few of the models are at present suitable for solving problems related to management and regulation. . . ., " in a review of potential uses of some leaching models for management and planning.

Optimizing N management has become important in recent years because dramatically increasing nitrate levels in groundwater have been attributed to crop N mismanagement. While this is not always the case, improvement in N management is needed to minimize nitrate leaching. Precision agriculture has developed rapidly over the past few years. Precision nitrogen management needs to consider optimization technologies, which challenge traditional N models. Nitrogen models are now required not only to describe the situations, but also to find optimal management strategies that reduce nitrate pollution while maintaining profits. In this chapter, the impact of management on the N cycle in soil-plant systems is first examined. Then, some existing optimization procedures related to management are discussed. Finally, Management-Oriented Modeling (MOM), a dynamic simulation modeling with artificial intelligence (AI) optimization techniques, is developed that searches for optimal N management to minimize nitrate leaching and maximize production and profits.

5-1. Optimization of Management

5-1.1. Management Changes the Fate of N

Nitrogen fertilizer application methods and timing have significant impacts on the fate of nitrogen in soil-plant systems. An appropriate N fertilization practice usually synchronizes the crop's requirement of N during crop growth, which supplies N when needed by the crop. This management practice uses N fertilizers effectively and reduces the risk of nitrate leaching. Mismanagement practices, such as applying N fertilizer in excessive amounts or mistiming, will increase the risk of nitrate leaching.

Although nutrient accumulation patterns vary among crops, major N uptake occurs during the rapid growth period for many crops. For example, a winter wheat crop takes up about 75% of its total N during its rapid growth phase (April to May) and a corn crop takes up 67% of its total N during its rapid growth period (July) in

Nebraska (Olson, 1978). A generalized pattern of N demand and uptake by a plant over time is derived from Fig. 4-2.5 and shown in Fig. 5-1.1. Generally a crop requires much more N during its flowering and fruiting stages than at the seedling and senescence stages. It is apparent that applying N fertilizer just before the time of most rapid N uptake will assure most effective utilization of N (Welch, 1971). Malzer and Graff (1984, 1985) compared grain yields of an irrigated corn with three fertilizer application methods (Fig. 5-1.2). The sidedress method had a high efficiency of N fertilizer utilization, the efficiency of preplant plus nitrification inhibitors was moderate, and the preplant method had the lowest efficiency. Low N fertilizer efficiency implies a higher risk of nitrate losses from the root zone because the nitrate remaining in a soil profile is exposed to the leaching potential of rainfall and irrigation. These examples of fertilizer timing show that nitrogen management plays a key role determining the fate of N in a cropping system.

Theoretically, if the N fertilizer supply can be synchronized with the plant needs as shown in Fig. 5-1.1, the maximum N fertilizer utilization will be reached and nitrate leaching will be minimized. Multiple applications with small amounts of fertilizer (e.g., split application) usually promote better plant uptake and reduce the potential of nitrate leaching as compared to a single application with a large amount of fertilizer (e.g., preplant application). The application rates, timing, and methods of N fertilizer and irrigation are important management tools that determine and control the fate and behavior of N in soil-plant systems. These tools can be used to adjust the rates of N release from the nutrient sources to match N availability with crop need. To perform

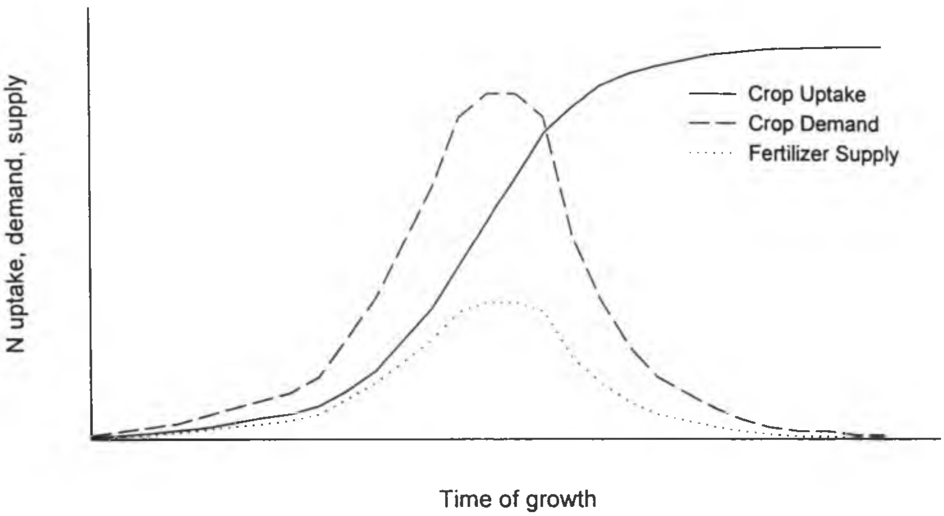

Fig. 5-1.1. Hypothetical crop N uptake-curve and N demand-curve. The rapid N uptake occurs at the period of the N demand peak. A hypothetical fertilizer supply synchronizes the crop N demand.

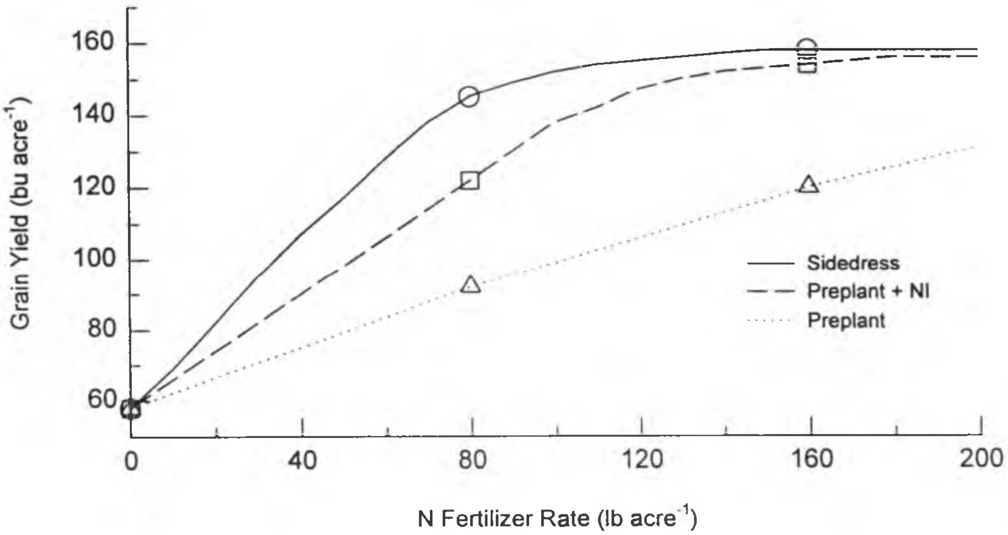

Fig. 5-1.2. An irrigated corn yields response to N fertilizer application timing and nitrification inhibitor (NI). Drawn from Malzer and Graff (1984, 1985).

precision nitrogen management, quantitative optimization techniques are usually involved in estimating application rates and timing of fertilizer and irrigation.

5-1.2. Linear Programming Models

Linear programming models are commonly used in the field of *management science* as a quantitative method for decision making. Among mathematical programming models, *Linear programming* is a special type in which objective function and all constraints are linear (Anderson, *et al.*, 1994). To optimize a static problem in N management, the linear programming would be a useful tool.

Suppose a static N model, QUEFTS, suggests a fertilizer requirement of 200 kg ha^{-1} N, 200 kg ha^{-1} P_2O_5, and 100 kg ha^{-1} K_2O for a crop. The available fertilizers are 11-52-0 (\$0.23 ha^{-1}) and 21-0-32 (\$0.17 ha^{-1}). The problem is to find the minimum amounts of the fertilizers that meet the nutrient requirements at minimum cost. In linear programming language, this is a minimization objective. Let

x_1 = amount of fertilizer 11-52-0 needed (kg ha^{-1})

x_2 = amount of fertilizer 21-0-32 needed (kg ha^{-1})

Then, the total fertilizer cost = $z = \$0.23\,x_1 + \$0.17\,x_2$

The objective is to minimize the cost, so

$$\min\ z = \min\ 0.23\,x_1 + 0.17\,x_2 \qquad [5\text{-}1.1]$$

where x_1 and x_2 are the decision variables. $0.23\,x_1 + 0.17\,x_2$ refers to the objective function. Because the combination of the fertilizers must satisfy the nutrient requirements, the amounts of the fertilizer supply follow the nutrient constraints:

for N $$0.11\,x_1 + 0.21\,x_2 \geq 200 \text{ (kg ha}^{-1}\text{)} \qquad [5\text{-}1.2]$$

for P_2O_5 $\quad 0.52\,x_1 \geq 200$ (kg ha^{-1}) [5-1.3]

for K_2O $\quad + 0.32\,x_2 \geq 100$ (kg ha^{-1}) [5-1.4]

$x_1 \geq 0, \quad x_2 \geq 0$ [5-1.5]

The above functions consist of a complete linear programming model for the fertilizer problem. Using a graphical solution procedure, the minimum cost of the fertilizers was found to be \$216 at the rates of 385 (kg ha^{-1}) for the 11-52-0 fertilizer and 751 (kg ha^{-1}) for the 21-0-32 fertilizer (Fig. 5-1.3). This example shows that linear programming solves optimization problems well for the static N management. Li *et al.* (1996) applied linear programming in selecting liming materials for acid tropical soils.

5-1.3. Dynamic Programming Approach

Although the linear programming models are useful optimization methods to solve many problems such as the example above, they become limited when the problems to be optimized are large and complex. For example, to determine an optimal management solution to minimize N leaching from a simple soil-plant system, an objective function may be given as a set of factors as follows:

N leaching = f (soil, weather, crop, management, time) [5-1.6]

where, arguments are also functions of other variables:

Soil = *f* {NO_3-*N(time)*, NH_4-*N(time)*, *OM(time)*, *moisture(time)*, *texture*, *pH*, *N transformations(time, soil properties)*}

Weather = *f* {*rainfall(time)*, *temperature(time)*, *ET(time)*}

Crop = *f* {*root uptake (time, rates)*, *rooting(depth)*}

Management = *f* {*fertilization(time, rates, methods)*, *irrigation(time, rates, methods)*, . . .}

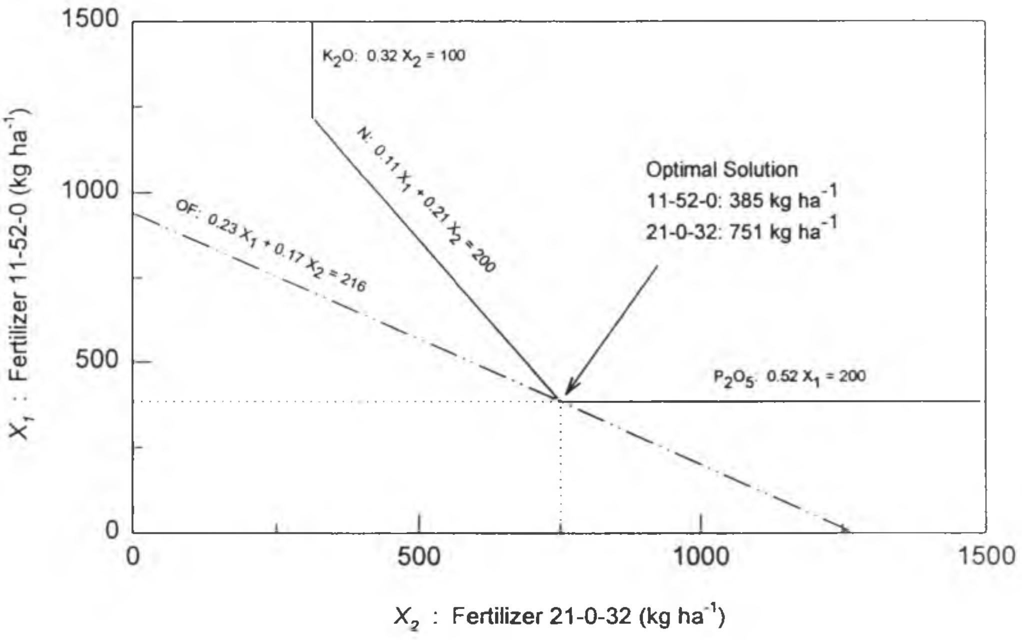

Fig. 5-1.3. Linear Programming Model for the fertilizer selection problem. The cost reaches the minimum of \$216 ha^{-1} at the optimal solution point.

For this type of complex problem, *dynamic programming* may be helpful. Dynamic programming is an approach to problem solving that permits decomposing a large problem that may be very difficult to solve into a number of interrelated smaller problems that are usually easier to solve (Anderson, *et al.*, 1994). Unlike linear programming as a specific algorithm, dynamic programming is a general approach to problem solving. Considering a large problem that can be divided into N subproblems (N stages), using dynamic programming notation, let

x_n = *input to stage n, state variable*

d_n = *decision variable at stage n*

x_{n-1} = *output for stage n (input to stage n-1), state variable*

The linkage of stage x_{n-1} to stage x_n is established by *stage transformation function* t_n:

$$x_{n-1} = t_n (x_n, d_n) \qquad [5\text{-}1.7]$$

So, the objective function can be given as

$$\sum t_n (x_n, d_n) \qquad [5\text{-}1.8]$$

This is an example of deterministic dynamic programming. Plant and Stone (1991) discussed the use of stochastic dynamic programming (called stochastic optimal control methods) to generate optimal irrigation schedules for a growing season. The schedules consist of daily stages. Using their notation, the decision variable is called control, u_k, which represents the amount of water applied on day k. The state variable x_k is a vector whose components represent the results of a simulation model for the crop-soil-water system. A dynamic programming model was abstractly given as

$$x_{k+1} = \phi_k (x_k, u_k) \qquad [5\text{-}1.9]$$

$$x_0 = a$$

where ϕ_k is called system dynamics that evaluates the state of the system from time k to $k+1$. The optimal control problem is to choose a sequence $\{u_1, u_2, \ldots, u_{D-1}\}$ to find optimal solutions to the problem by an objective function:

$$\sum \phi_k (x_k, u_k) \qquad [5\text{-}1.10]$$

If considering uncertainty, a stochastic dynamic programming model can be expressed as

$$x_{k+1} = \phi_k (x_k, u_k, \eta_k) \qquad [5\text{-}1.11]$$

$$x_0 = a + \omega$$

where η_k is a vector-valued random process representing the system "noise" on day k. ω refers to a vector representing the uncertainty in the initial conditions. No implementation for the model was discussed. The application of optimization techniques to irrigation scheduling has been researched by many investigators (Dudley *et al.*, 1971; Hall and Butcher, 1968; Rhenals and Bras, 1981; Yakowitz, 1982). However, only few successful implementations in agriculture have been reported. Plant and Stone (1991) concluded some problems associated with the implementation in agriculture: (1) the accuracy of the system model may be insufficient; (2) the model parameters are difficult to estimate for specific cases; and (3) the model computations become intensive with stochastic situations.

5-1.4. Knowledge-Based Systems Embedded in Simulation

A primary advantage of computer simulation is its applicability in complex situations where analytical procedures are difficult. Computer simulation can be used to obtain dynamic information such as N leaching expressed by equation [5-1.6]. Actually, computer simulation models and their programs provide convenient laboratories for experiments in many fields. With these laboratories, preliminary experiments become easy to conduct. However, simulation models cannot guarantee an optimal solution to a problem. Although decision makers can run the computer simulation long enough to try all possibilities of their decision variables, it may be too costly or require too many resources to solve the problem. In many cases, this method is impossible to perform because the running time may be too long to be acceptable, or the values of decision variables become nearly infinite.

Schaub and Stone (1989) developed an example of integrating simulation models with expert systems to form hybrid systems. The system was used to find nearly optimal strategies represented by a set of rules for the pest control in cotton fields. This hybrid system consisted of three independently developed biological simulation models (Gutierrez *et al.*, 1984; Richardson and Wright, 1984; Sequeira *et al.*, 1989) linked to a rule-based system (Fig. 5-1.4). For each simulation day, the random weather generator, WGEN, produces daily temperature, rainfall, and solar radiation. The cotton model simulates the cotton growth and development as influenced by weather. The bollworm model simulates immigration and development of bollworms in cotton fields which are subject to weather, natural enemies, and management actions. The rule-based system, Management Model written in the LISP language, uses the output of the simulation models to determine future courses of the simulation. With AI search methods, a heuristic optimization procedure, called *heuristic programming*, was developed to find nearly optimal rules for the pest control (Stone and Schaub, 1990).

This hybrid system was not developed to directly give advice to a farmer for a specific cotton field. The knowledge-based system was embedded in the simulation model as an analysis tool to determine which pest control strategies were better overall. The possible pest control strategies were tested using the hybrid system. Ultimately, nearly optimal pest control strategies were elicited from the analysis and added into a rule-based system as a set of decision rules, which were used by farmers to make their

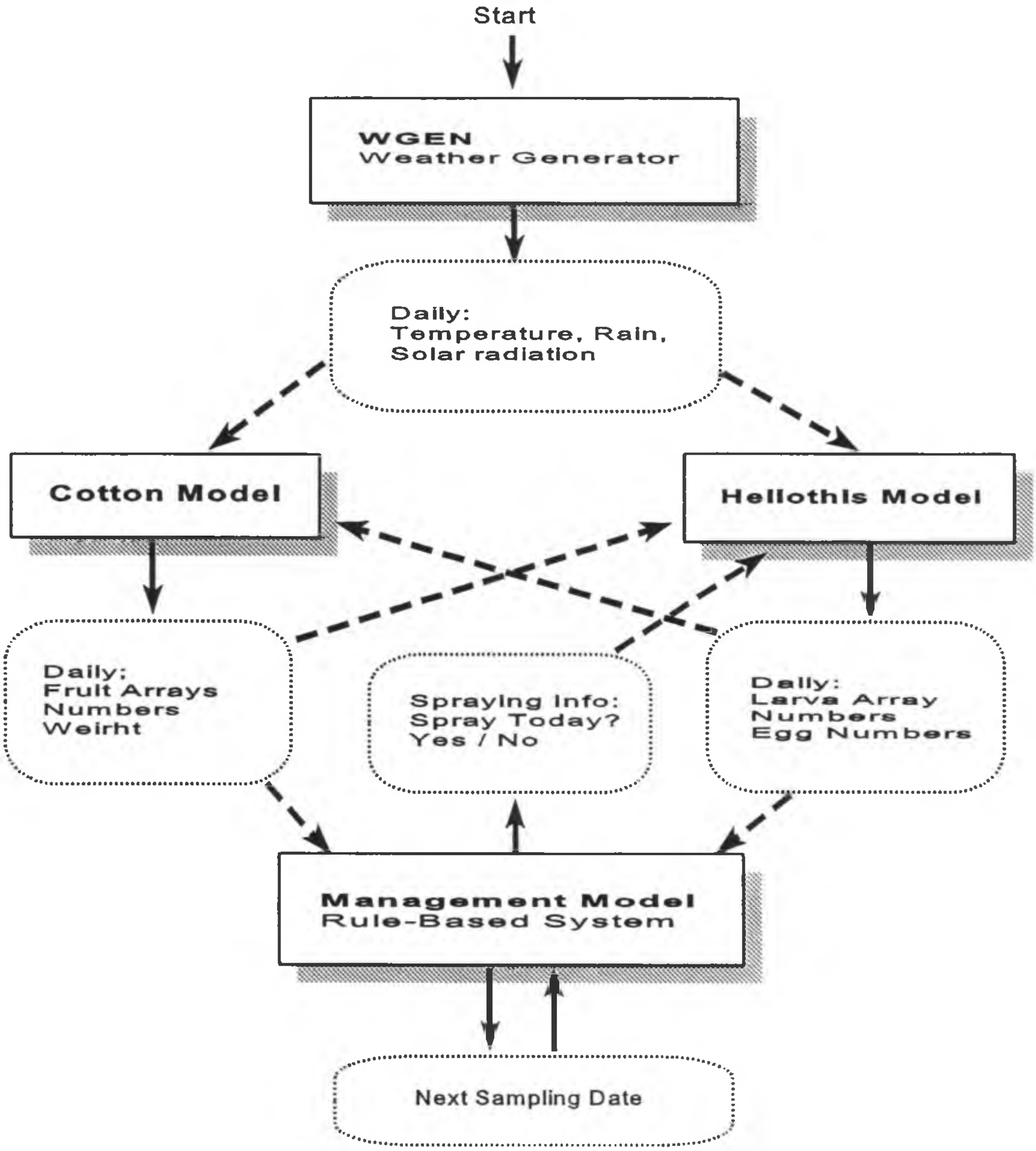

Fig. 5-1.4. Linkage among the components of the hybrid knowledge-based system and simulation models of Helicoverpa spp. and Cotton. Source: Stone and Schaub, 1990.

decisions in particular situations (Plant and Stone, 1991). This is a good example of using knowledge-based systems to control simulation models.

5-2. MOM Structure and Characteristics

Linear programming is a useful method to optimize static N management problems. The dynamic optimization approach and simulation models with AI techniques provide precision technologies with the dynamic N management. However, simulation models with AI optimization for dynamic precision N management have not been reported. This study was conducted to explore a modeling approach that constructs simulation models using AI optimization methods for precision N management. The specific objectives were:

(1) Develop a management-oriented algorithm that directs the simulation model toward user-weighted goals. There are many users' goals for cropping, such as maximizing product quality, appearance, nutrient content and others. The model takes three goals (objective functions) as examples in this study: minimizing nitrate leaching while maximizing crop yields and profits.

(2) Develop an optimization algorithm that can specify a range in management variables in which optimal solutions are guaranteed. The model searches for solutions only around this range instead of all possible solutions. This algorithm is critical to ensure that the model solves problems in a small amount of time which is acceptable for users to implement the model on current personal computers.

(3) Design this dynamic optimization model for multiple purposes and users. The model can be used as a tactical N management tool for specific conditions and be used as a strategic N management tool for general decision rules. The model will be constructed as a useful tool for diverse users from farmers to scientists.

5-2.1. MOM Structure

As discussed in section 5-1.4, computer simulation models are convenient laboratories to conduct experiments. To conduct a field experiment of fertilizer rates with irrigation, for example, it will take a cropping season, usually a couple of months. The experiment can also be conducted using computer simulation models in a few minutes at much less cost if the models are validated for the conditions of the field experiment. The process of computer models that mimic the field experiments to find optimal management strategies can be illustrated by a simple example called "burgling a safe" using *generate-and-test* method in artificial intelligence (AI) (Winston, 1992). To try a three-number and two-digit safe, one can start with the combination 00-00-00, move to 00-00-01, then 00-00-02, and continue on through all possible combinations until the door opens. In terms of AI, the counting is called the generation procedure and the twisting the safe handle is called the testing procedure. One of the great classic application programs using this AI technique is DENDRAL (Winston, 1992). It was used to identify the structure of an organic chemical by comparing the real mass spectrogram with those produced by the computer generator.

To construct a computer model to conduct the experiment of fertilizer and irrigation rates, for example, the procedure of designing treatments in the experiment seems as the "generator" and analyzing results of experiment as the "tester" in the *generate-and-test* method. Then the treatments are put in a laboratory to conduct the experiment, which examines the responses of soil-plant systems. The laboratory is a computer simulation model called a simulator. So there are three components, a generator, a simulator, and an evaluator, involved in the experiment conducted by the computer simulation. In general, the generator produces the combinations of management strategies (e.g., the treatments of fertilizer rates plus irrigation rates in the example above). The simulator executes the management strategies and simulates their effects on a soil-plant system such as nitrate leaching, crop yields and profits. The evaluator examines the simulation results to find which management strategy produces a better result (e.g., less nitrate leaching, higher yields and profits). If one wants to find optimal combinations of fertilizer rates plus irrigation rates, the evaluator information can be fed back to the generator to adjust the rates of the fertilizer and irrigation. Then repeat the experimental procedures described above. The experiment is conducted by the computer models using a ***generator-simulator-evaluator*** procedure. Since this modeling approach concentrates on optimizing management strategies, we call it as **Management-Oriented Modeling (MOM)**. The MOM structure is shown in Fig. 5-2.1. We first describe MOM structure and its characteristics of mimicking human actions in N management, then discuss MOM implementation in detail in section 5-3.

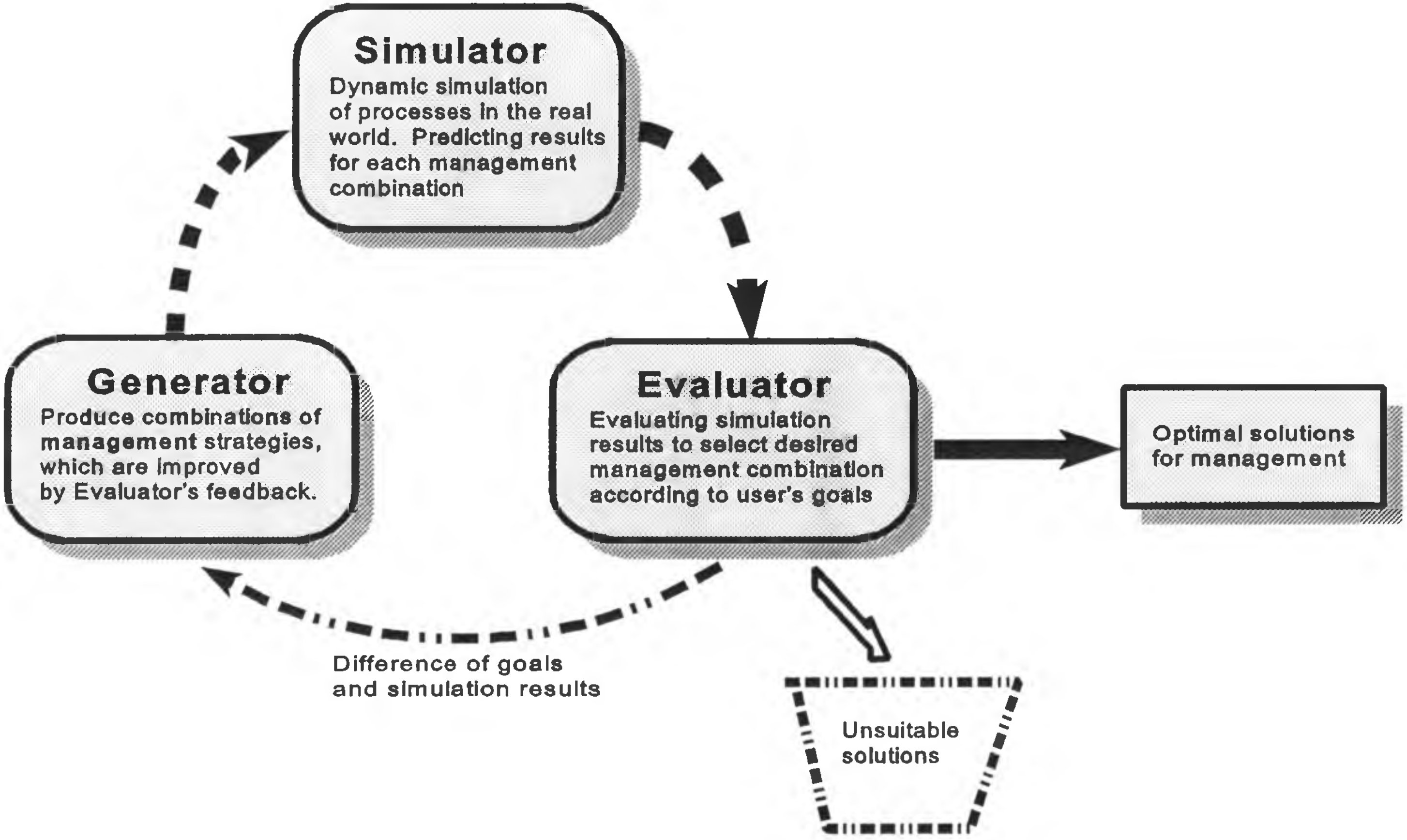

Fig. 5-2.1. Diagram of Management-Oriented Modeling Structure

5-2.2. Two-Way Modeling

There are two ways for decision-makers to interact with the real world. First, the world is mapped to decision-maker's brain where decision-makers describe and understand the real world by the "maps" of the real world. Second, after the understanding, decision-makers make some "modifications" to control and change the real world (Fig. 5-2.2). As the discussion in the Chapter 3, many existing N simulation models simulate the N cycle in soil-plant systems based on inputs of soil, plant, weather and management data. This is an important type of modeling, ***description***. In addition to ***description***, MOM is designed to model decision-maker's *modification* of the real world. In other words, MOM not only simulates natural processes of the real world, but also simulates human actions on the real world to find possible optimal "modifications." We call this modeling approach two-way modeling. After analyzing "native" situations (without the fertilization and irrigation) of a soil-plant system, MOM selects a management action of fertilization and irrigation to "modify" the "native" situations. Then the management effects on the soil-plant system are evaluated to determine if they are improvements toward optimal management strategies. If no optimal management strategies are reached, MOM improves the management strategies and repeats the simulations to assess the management effects. MOM continues to repeat alternately between the two ways of modeling as the processes above until optimal management strategies are found (Fig. 5-2.2).

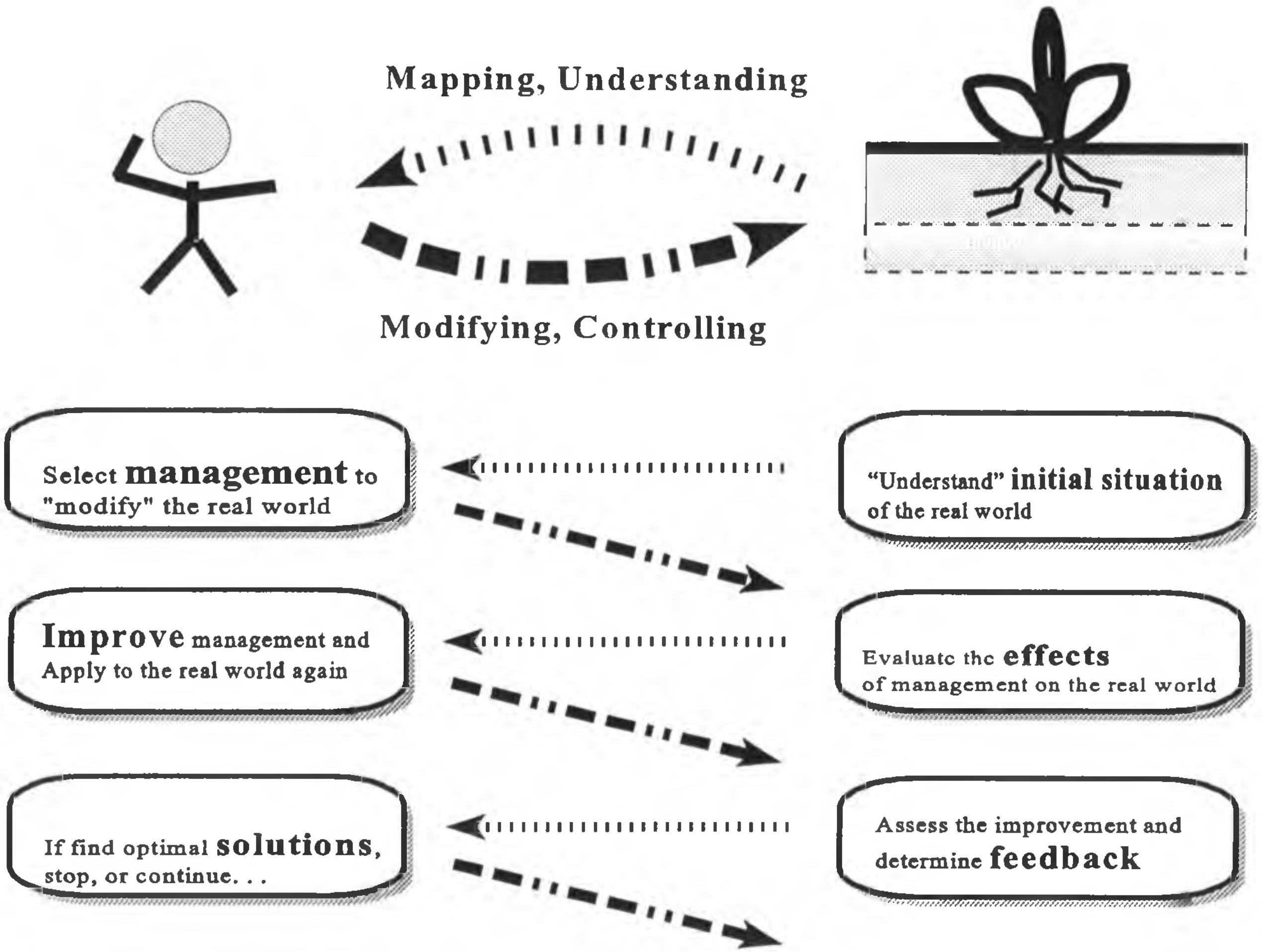

Fig. 5-2.2. Diagram of the Two-Way Modeling between human actions and natural processes of the real world.

5-2.3. Goal-Driven Modeling

Traditionally simulation models were driven by data. In other words, users input data and models output answers. Taking an example of reducing nitrate leaching during cropping, the modeling starts from the management practices under given local natural conditions and outputs predictions of crop yield and N leaching. The **solutions** are **crop yields** and **leachate nitrate**. The modeling processes are driven by data including management practices. We call this *Data-driven* modeling. The number of input datasets determines how many answers the models output (Fig. 5-2.3). In many circumstances of N management practices, however, people want N models to assist in finding optimal management strategies that are better than current ones, instead of only an assessment of the current practices. For these situations the model **solutions** become **management strategies**. To solve this kind of problem, the modeling can start from goals, high crop yields and low nitrate leaching, for example. Then it simulates the possible management practices under given local physical conditions and outputs optimal management strategies that can reach the goals (Fig. 5-2.3). The modeling direction is reversed from the traditional simulation modeling. In the MOM modeling, the amount of management data needed depends upon the goals. MOM only chooses management strategies that produce the results toward the goals to simulate. We call this modeling as *Goal-driven* modeling. This *Goal-driven* simulation is one way Management-Oriented Modeling differs from the traditional simulation models.

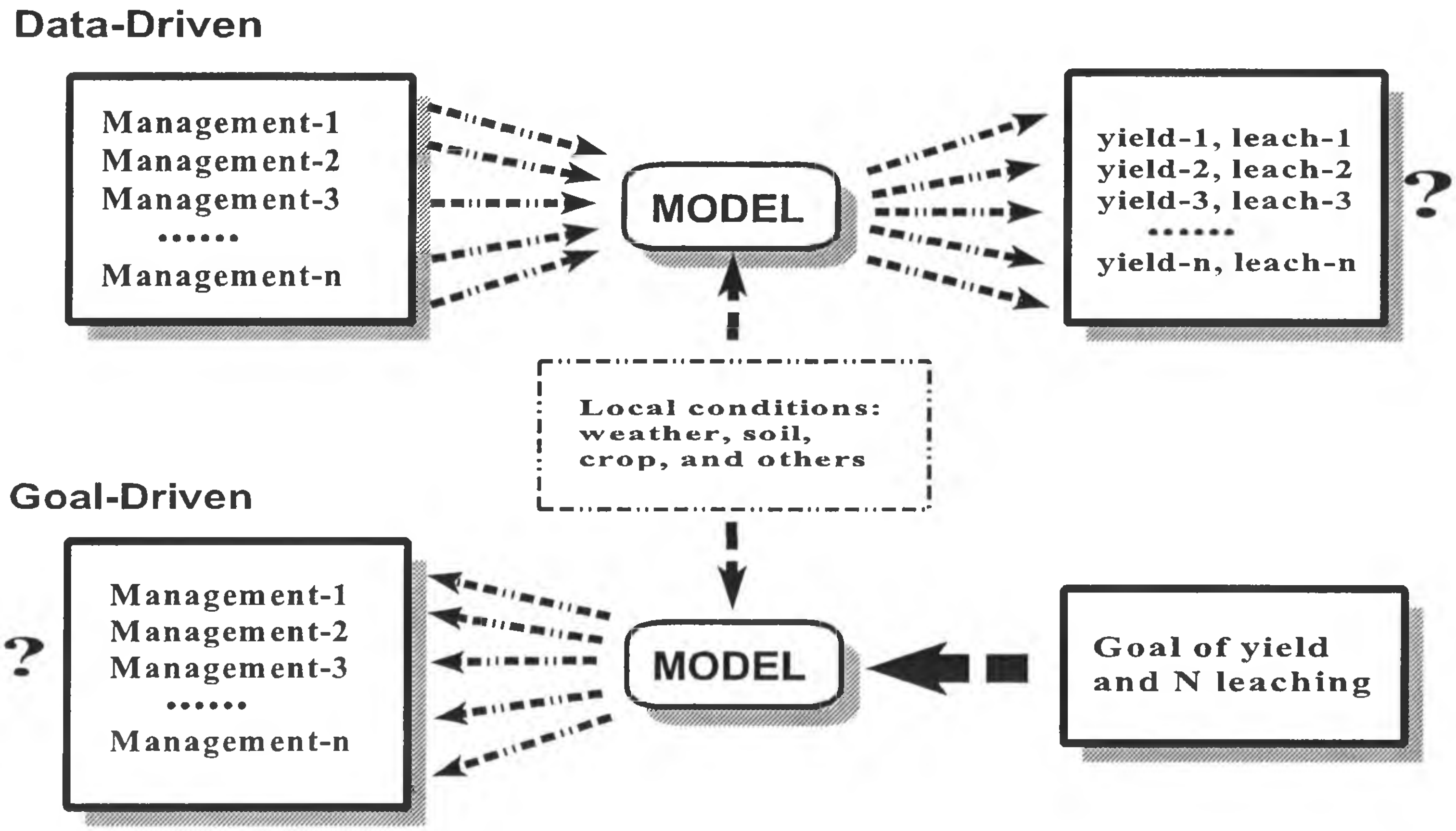

Fig. 5-2.3. Diagram comparing Data-driven modeling with Goal-driven modeling.

5-2.4. Multiple Solutions

In reality, there may be multiple solutions for a goal. For example, among all possible combinations of the N management strategies, some combinations with different fertilizer and irrigation rates may result in approximately the same yield and/or nitrate leaching (refer to Fig. 5-2.3). In other words, MOM may find multiple answers for a goal without changing the data inputs and given physical conditions. This characteristic provides users with opportunities to choose the most suitable solution among a group of answers to match their particular situations. It also offers users alternative solutions if their situations change.

5-3. MOM Implementation

The MOM implementation will be discussed following its *generator-simulator-evaluator* structure (Refer to Fig. 5-1.5).

5-3.1. Knowledge Representation in MOM

Good implementation starts from a good knowledge representation. The representation principle says "once a problem is described using an appropriate representation, the problem is almost solved" (Winston, 1992). To solve the problems of N management using AI techniques, the major task is to appropriately represent the knowledge of the N management with AI languages. Assume that a set of management strategies are consisted of N fertilizer applications and irrigations of various rates and timing. Each management strategy produces a profit, a crop yield, and an N leaching rate (Table 5-3.1). MOM's task, for example, is to find which management strategy produces a maximum crop yield and profit with a minimum N leaching, among the seven strategies in this hypothetical example.

Table 5-3.1. Hypothetical management strategies and their simulated results.

Management Strategy #	N Fertilizer Rate *kgN ha⁻¹*	N Fertilizer Timing *Apps.†*	Irrigation Rate *mm*	Irrigation Timing *Apps.‡*	Profit *\$ ha⁻¹*	Yield *kg ha⁻¹*	Leachate N *kgN ha⁻¹*
#1	80	14	407	2	461	7480	40
#2	80	14	136	2	475	7486	0
#3	80	2	271	2	685	7797	15
#4	160	14	407	7	742	10399	37
#5	240	2	136	2	759	8611	0
#6	240	14	271	7	802	11003	8
#7	240	2	271	2	976	10881	8

† Number of N fertilizer applications during the cropping season.
‡ Number of irrigation days a week.

To illustrate a visual concept of the AI representation for this example, the profits against leachate N were plotted in Fig. 5-3.1. The points (circles) in Fig. 5-3.1 represent the N management strategies (rates of fertilizer and irrigation) in Table 5-3.1, which are called **nodes** [1] in terms of AI language. The result (the crop yield, profit and leachate N) of each corresponding management strategy is called the **state** of the node. To perform MOM's task, finding a better management strategy, one just goes over the results of the management strategies one by one until the answer is found. The process of examining the results to find solutions is called **search**. During the search, a move from one node to another is called a **link** or **path** between the nodes. A path or link denotes a transition between states, actually a change of the management strategy from one to another in MOM. The nodes linked by paths form a **semantic net**. It is also

[1] See Glossary for more information of AI terminology.

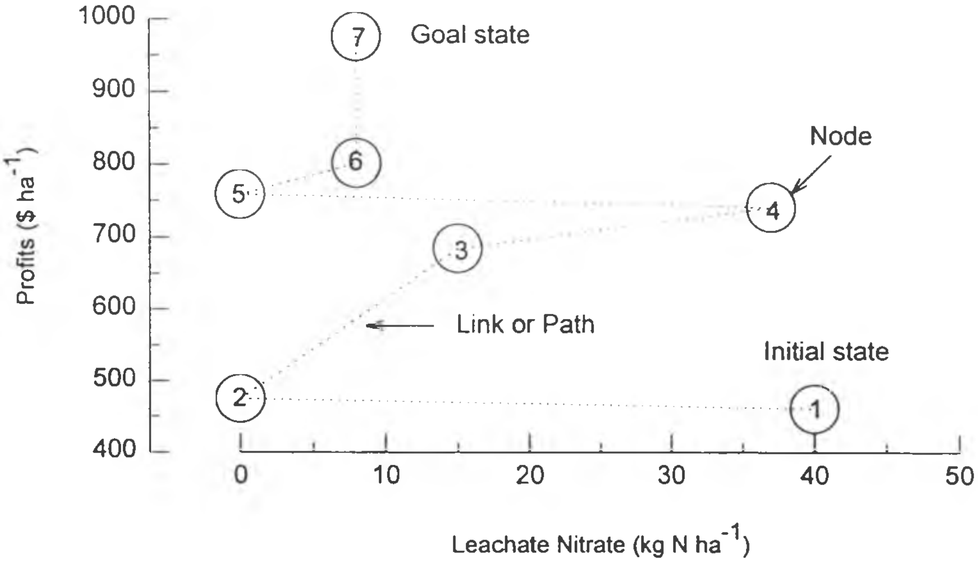

Fig. 5-3.1. Knowledge representation in MOM with AI language. The state space consists of nodes linked by paths. The states of the nodes are denoted by their positions in the space with dimensions of profits versus leachate nitrate.

called a **state space** in which the states of nodes were represented by their positions in the two-dimension space (profits versus leachate N in MOM). The search objective, an optimal management strategy in this example, is called a **goal**. The node that satisfies the goal is called a goal node. The state of the goal node, characterized by a minimum of N leaching and maximum of the yields and profits in this example, is also called as goal in following discussion. So the goal in MOM consists of three sub-goals: minimizing N leaching, maximizing yields and profits. MOM's task, in AI language, is finding goal nodes. Comparing the profits, yields, and leachate N of all management strategies, the states of the nodes of strategy #6 and #7 (Table 5-3.1), for example, are closer to the goal state than others. If three sub-goals are of the same importance, an overall nearly optimal solution among the strategies is management strategy #7 for this example.

5-3.2. MOM Generator

The MOM generator is designed to produce the N management strategies consisting of the rates and timing for N fertilizers and irrigation. Winston (1992) suggested that a good generator usually has three properties: complete (eventually producing all possible solutions), nonredundant (never compromise efficiency by proposing the same solution twice), and informed (use possibility-limiting information, restricting the solutions that they propose accordingly). In this section, we discuss how the MOM generator uses the knowledge of the N cycle in soil-plant systems to prune redundant nodes, while ensuring that the goal nodes are within a limited range to be searched.

5-3.2.1. Combinations of Management Strategies

Recalling the example of "burgling a safe" in section 5-2.1, the total combinations for the safe of three-number with two-digit are 100^3 = one million. The situation of N management is much more complicated than this example. Among the N management factors, the rates and timing of N fertilizer and irrigation are chosen to test the MOM concept in this study -- which are important the factors in controlling the fate of N in soil-plant systems. Changing these factors will change crop yields, profits, and nitrate leaching rates, which are the goal states of three sub-goals in MOM. Consider N management practices that specify fertilizer rates and irrigation rates which are split during the cropping season. An N management strategy in MOM consists of three factors: *fertilizer rate, irrigation rate, time* (when fertilizer or irrigation applied). It can be expressed as

$$M_i = f\,(fertilizerRate_i\,,\ irrigationRate_i\,,\ Time_i) \qquad [5\text{-}3.1]$$

where M_i is a management strategy in MOM ($i = 1, 2, 3, \ldots \infty$). Theoretically there are an infinite number of combinations of management strategies. To simplify the situation by considering only three rates for N fertilizer and three rates for irrigation during a 140-day cropping season, the problem becomes one of finding an optimal management combination among three N fertilizer rates combined with three irrigation rates scheduled during 140 days. The number of combinations from the fertilizer rates and the irrigation rates with a time factor can be calculated by

$$Combinations = (fertilizerRates \cdot irrigationRates)^{\,time} \qquad [5\text{-}3.2]$$

It implies that the number of management combinations in dynamic systems will increase exponentially because of involving the time factor (when applying fertilizer and water in MOM). For this instance, the management strategies for scheduling one day are nine combinations ($3 \cdot 3 = 9$). However, the number of combinations for two days is $9 \cdot 9 = 81$, and $9^3 = 729$ for three days. The total number of the combinations for a 140-day cropping is $9^{140} \approx 4 \cdot 10^{133}$. Reducing the time steps to weekly, the total number of the combinations is $9^{20} \approx 10^{19}$, still an astronomical figure. An N management problem is thus far more complex than the "burgling a safe" case. Assuming the simulation of the N cycle in a soil-plant system for a growth season can be finished in 0.001 second, it will theoretically take about $3 \cdot 10^8$ years to examine all combinations without accounting for the time of search in the computation.

5-3.2.2. Prune Unnecessary Combinations

Facing the challenge of the huge combinations, the first task for the MOM generator is to reduce the large number of the combinations to a reasonable range in which the most promising combinations are included. The most unnecessary combinations can be pruned by analyzing the real situation of the soil-plant system relevant to MOM. In an example of tomato N fertilization experiments (Fig. 5-3.2a), the crop yield increased with increasing N fertilizer rate until a yield plateau (point B in Fig. 5-3.2a) was reached. The risk of potential nitrate leaching (represented by *Excess N* in soil profiles, Fig. 5-3.2a) was very low when N fertilizer rate was less than the maximum (plateau) crop requirement (point B in Fig. 5-3.2a). After N supply exceed the crop maximum requirements, the risk of potential nitrate leaching increased proportionally. Same analysis can be applied to irrigation rates. For an upland crop, the yield response to increasing water supply may increase at first to a peak, then drop down gradually because of oxygen stress. A general situation of N fertilization with irrigation for a up-land crop was summarized in Fig. 5-3.2b. The figure implies that there exists a range (between point “A” to point “B” in Fig. 5-3.2b) in which the N fertilizer and irrigation rates are close to the crop requirements. Within the range, the optimal solutions for the MOM goals, maximizing crop yields and minimizing nitrate leaching, should be included. The range is the area labeled from the point “A” to point “B” in Fig. 5-3.2b, called the **promising solution zone** in MOM. In other words, the management nodes outside of the promising solution zone can be considered as unnecessary combinations and should be pruned. To eliminate unnecessary

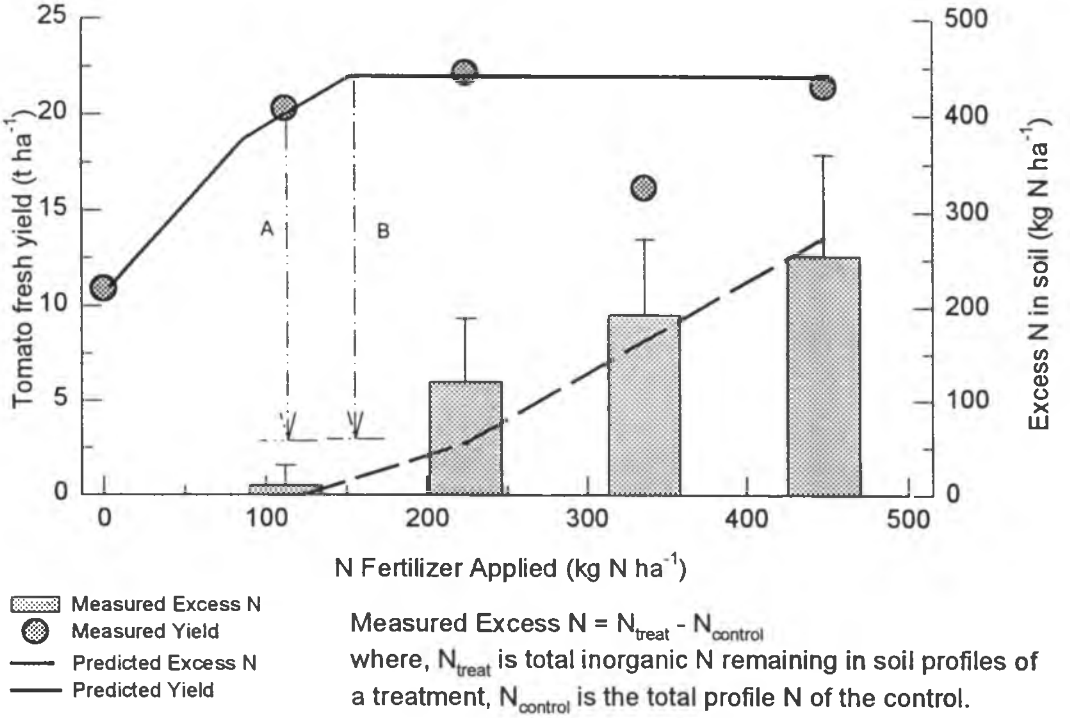

Fig. 5-3.2a. N-BALANCE model predicted and measured tomato yields and Excess N remaining in soil with changes of N fertilization rates. Source: Yost *et al.*, 1997b.

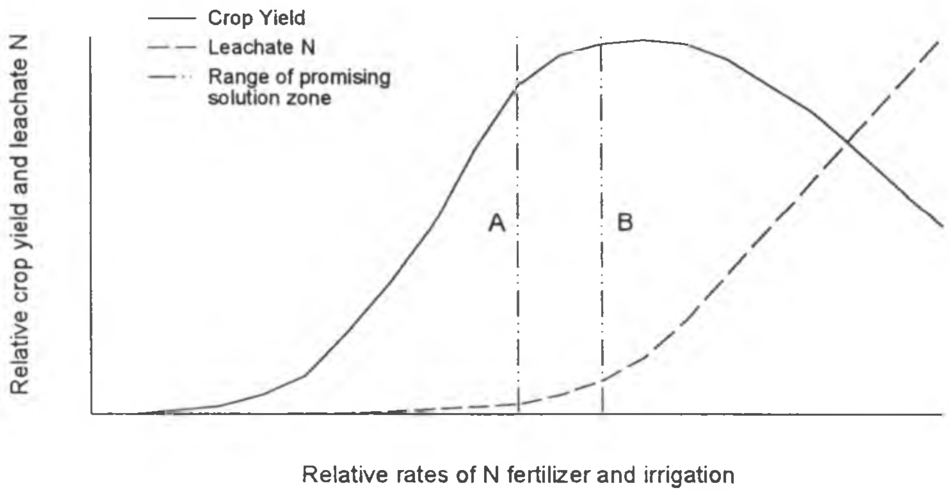

Fig. 5-3.2b. The N fertilizer and irrigation rates within promising solution zone (range between point "A" and point "B") nearly match the crop requirements. The optimal solutions for the MOM goals should be included in this zone.

management combinations, the MOM generator needs a procedure to identify the promising solution zone for each specific situation.

5-3.2.3. Analyzer of Soil N and Water Supply Potentials

The daily crop requirements of N and water change during growth. MOM needs a dynamic simulation analysis to trace this situation. A situation analyzer, the algorithm estimating soil N and water supply, is developed for the MOM generator to analyze the crop dynamic differences between the requirements and soil supplies. In the analysis procedure, MOM generator first detects the "native" supply potentials of soil N and water by calling N-SIMULATOR (See chapter 4) in the *background* mode (the simulation without N fertilizer and irrigation, see section 5-3.3). This simulation records soil moisture and soil mineral N content for each growing day. Then daily soil water supply potential can be estimated by soil water supply index, $SupIx_{water}$

$$SupIx_{water} = \log \frac{\theta_{Actual} - \theta_{PlantLmt}}{\theta_{PlantGoal} - \theta_{PlantLmt}} \qquad [5\text{-}3.3]$$

where θ_{Actual} is the actual soil water content without irrigation at a simulation day. $\theta_{PlantLmt}$ is the soil water content at the low plant extractable limit. $\theta_{PlantGoal}$ is the soil moisture goal that a crop requires. $\theta_{PlantGoal} = K_{\theta goal} \cdot \theta_{DrainLmt}$. $\theta_{DrainLmt}$ is the soil water content at the drained upper limit (Refer to section 4-2.2). $K_{\theta goal}$ (0-1) is a coefficient of expected soil moisture for a specific crop. $K_{\theta goal}$ is used to adjust the soil moisture goal. If a crop requires soil moisture at $\theta_{DrainLmt}$, $K_{\theta goal} = 1.0$. If a crop requires soil moisture as a half of $\theta_{DrainLmt}$, $K_{\theta goal} = 0.5$. The soil water supply index, $SupIx_{water}$, can be used to flag the soil water supply to a crop:

If $SupIx_{water} = 0$, the soil moisture satisfies the crop requirement.

If $SupIx_{water} < 0$, the soil moisture does not satisfy the crop requirement.

If $SupIx_{water} > 0$, the soil moisture exceeds the crop requirement.

The daily soil N supply potential is estimated by soil mineral N supply index, $SupIx_N$

$$SupIx_N = log\ (F_{root} \cdot N_{supply} / N_{plantDemand}) \qquad [5\text{-}3.4]$$

where $N_{plantDemand}$ is the amount of N a plant demands (refer to equation [4-2.6]). N_{supply} is soil N supply potential (Refer to [4-2.7]). F_{root} is a root density fraction (Refer to [4-2.9]). The interpretation of $SupIx_N$ is similar as $SupIx_{water}$:

If $SupIx_N = 0$, soil N supply is sufficient for the crop.

If $SupIx_N < 0$, soil N supply is not sufficient for the crop.

If $SupIx_N > 0$, soil N supply exceeds the crop requirement.

Examples of the analyses of soil mineral N and water supply potentials during a cropping season are shown in Fig. 5-3.3.

5-3.2.4. Generate Primary Management Schedule

The above analyses provide the generator with the dynamic estimation of the shortages of soil N and water supplies. To estimate the amounts of N and water needed on a growing day, the MOM generator compares the amounts of N and water that a crop demands with the soil N and water supply in the "native" situation. The daily water needs, W_{need} *(mm)*, is calculated by

$$W_{need} = 10\ (K_{\theta goal} \cdot \theta_{DrainLmt} - \theta_{Actual}) \cdot Lyr + ET - Rain \qquad [5\text{-}3.5]$$

where $K_{\theta goal}$, $\theta_{DrainLmt}$ and θ_{Actual} are the same as in equation [5-3.3]. *Lyr (cm)* is the thickness of a root zone. The daily N needs, N_{need} *(kg N ha⁻¹)*, is calculated by

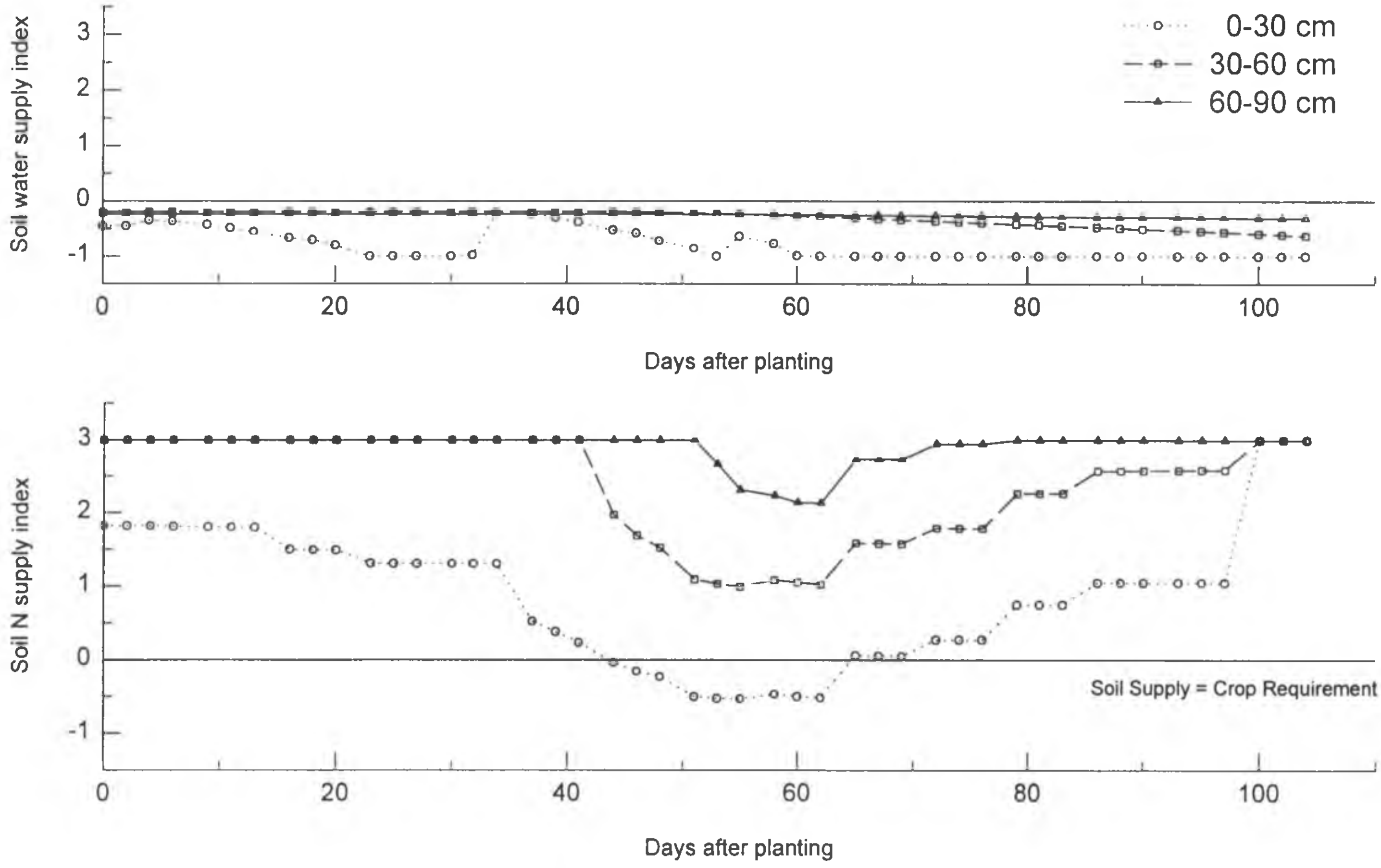

Fig. 5-3.3. The analysis diagrams of soil water and nitrogen supply potential. The supply indexes in three soil layers show that there existed water and N shortages in the surface soil layer in this example.

$$N_{need} = (N_{plantDemand} - N_{uptake}) / E_{fert} \qquad [5\text{-}3.6]$$

where $N_{plantDemand}$ *(kg N ha^{-1})* is maximum N the crop requires and N_{uptake} *(kg N ha^{-1})* is the N that the crop absorbs, without applied N fertilizer, on the current simulation day or week. E_{fert} is the efficiency of N fertilizer utilized by the crop (Yost *et al.*, 1997a).

With equation [5-3.5] and equation [5-3.6], the generator determines approximate amounts of N and water needed (the implementation is calling *DetectWater* and *DetectNitrogen* simulation modes, will be discussed in section 5-3.3). Then MOM generator produces a primary management combination, a schedule of N fertilization and irrigation during the cropping. This management combination should fall within the *promising solution zone*, the range from the point "A" to point "B" in Fig. 5-3.2b. An example of a primary management combination in week steps is shown in Fig. 5-3.4. Around this primary management schedule, the generator produces the first group of the management combinations by extending the primary rates of N fertilizer and irrigation. How the generator improves its following generations of the management combinations will be discussed in section 5-3.4, MOM Evaluator. Now the management strategies can be used by other two MOM components, the simulator and the evaluator.

5-3.3. MOM Simulator

To implement Management-Oriented Modeling, the MOM simulator is designed by extending the running modes of the dynamic simulation model, N-SIMULATOR that was constructed in chapter 4. As the MOM simulator, N-SIMULATOR operates in a MOM session in six simulation modes: *Validation,*

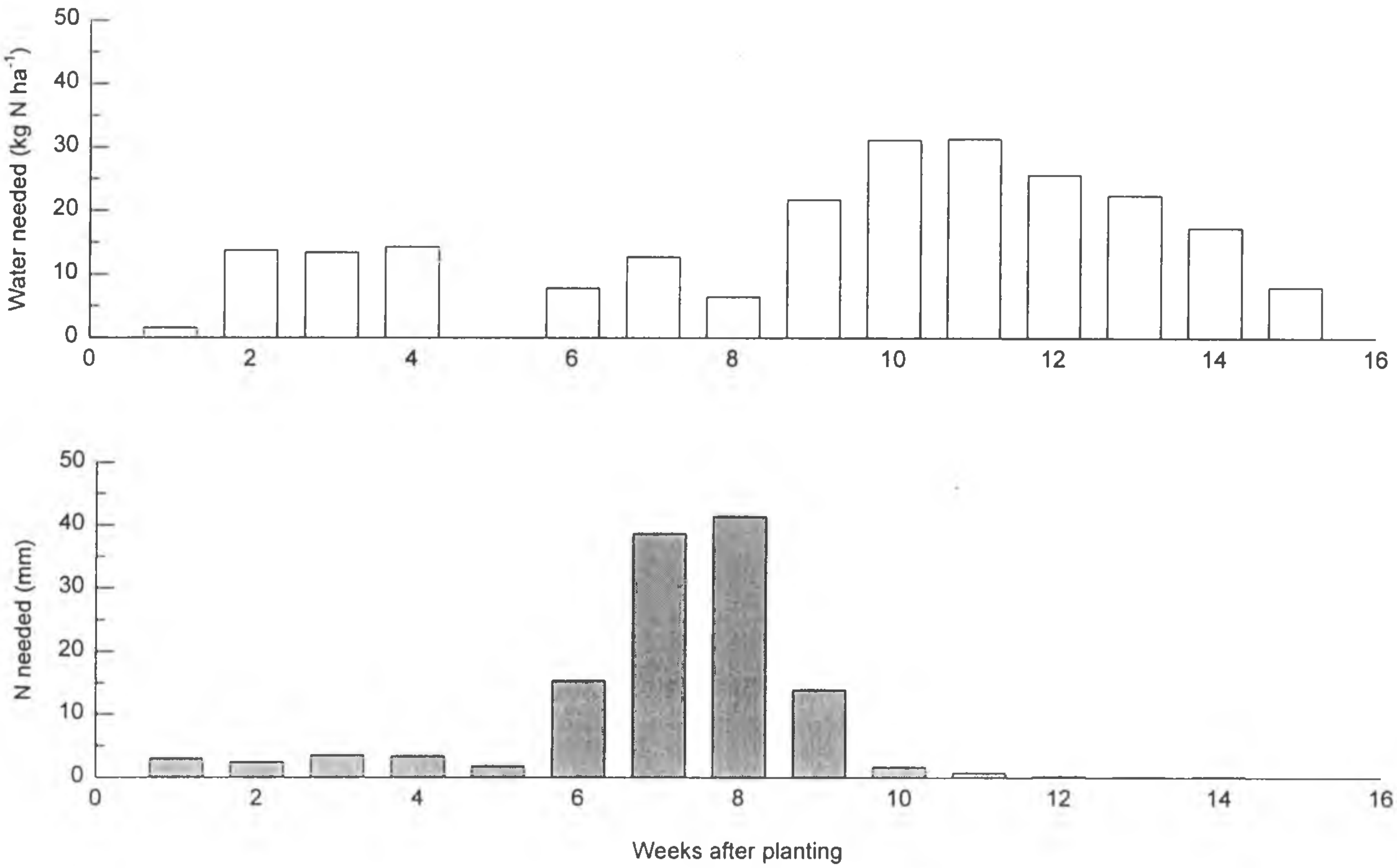

Fig. 5-3.4. A primary management combination in week steps, the schedule of N fertilization and irrigation, is produced by MOM generator. The schedule nearly synchronizes the crop requirements during the growth.

Background, DetectWater, DetectNitrogen, Optimization, and *PredictGrowth*. The characteristics of the modes are discussed below.

5-3.3.1. Validation Mode

Validation mode is the N-SIMULATOR itself without any change. The primary purpose of this mode is designed for users to calibrate the MOM simulator parameters to their specific site situations using their datasets. This mode also provides users with opportunities to use the MOM as a traditional simulation model for any other purposes. The default outputs of the *Validation* mode are database files and screen graphics. The graphic outputs are used to analyze the simulation results immediately during the simulation. They include daily outputs of soil water and N supply potentials, infiltration, fertilization, crop N uptake, leachate nitrate, soil nitrate content and soil ammonium content in three soil layers during the cropping season. The database files are Paradox format that can be retrieved by spreadsheets such as Quattro Pro, and used for users' specific analysis or assessment. The default outputs in the database files include runoff, infiltration, waste irrigation N, fertilizer N, top biomass N, root N, leachate nitrate, denitrification N, and soil layer data of nitrate, ammonium, soil moisture contents, and organic N released from several pools such as soil organic matter, organic wastes, and waste irrigation.

5-3.3.2. Background Mode

A "native" situation in MOM means that there have been no applications of N fertilizer and irrigation during a simulation. All other management activities are included in the "native" situation such as pest control and preplant organic residues, which are treated as natural conditions such as rainfall in MOM sessions. The *Background* mode ignores the fertilizer and irrigation applications in the data inputs and has the same outputs as the *Validation* mode. This mode is primarily designed as a tool to analyze a "native" situation for a MOM session. This background information is used to determine what amount of N and water are needed and when they are applied as users adjust the management strategies manually. This mode is also useful for a strategic management planning before cropping even if users do not use MOM sessions.

5-3.3.3. Detect Water, Detect Nitrogen Modes

The specifications of the *DetectWater, DetectNitrogen* modes are described in section 5-3.2.4 and their implementations are discussed in this section. Since the "native" situation would change with any application of fertilizer or irrigation, equation [5-3.5] and equation [5-3.6] cannot be statically used to calculate the N and water requirements based on the initial situation. For example, if the fertilizer or irrigation is applied in a day, the situations of following days are no longer "native." Assuming there exist N and water shortages on 7th and 8th weeks in a "native" situation and then N fertilizer and water are applied on 7th week, for example, the original shortages on 8th week may decrease or disappear. Therefore, the effects of the N and water applications in a previous week must be accounted for in estimating the requirements of N and water for following weeks, when determining the primary management strategies based on the "native" situation.

In *DetectWater* mode, MOM assumes that the crop grows normally without N deficiency, and that normal evapotranspiration of the soil-plant system will prevail during the cropping season. At the beginning of a simulation week, the MOM simulator first estimates the amount of water needed this week by accumulating the amount of water shortage in soil layers using equation [5-3.5]. Then the simulator applies this amount of water to the soil during the daily simulation for this week, on the week days that users scheduled. The applied water will change soil moisture of this week. This changed soil moisture will be used to estimate the amount of irrigation for the following week by equation [5-3.5]. At the beginning of the following week, the simulator estimates the irrigation amount again, and then repeats the above processes week by week. Finally the simulator determines weekly water requirements, or a primary irrigation schedule, for the cropping season (Fig. 5-3.4). Based on this irrigation schedule, the simulator switches to estimate the N requirement in the *DetectNitrogen* mode.

In the *DetectNitrogen* mode, the implementation procedure is different from that in the *DetectWater* mode. In the *DetectWater* mode, the water requirement of a week can be determined before the beginning of the week simulation because all items in the equation [5-3.5] have been known in advance. But the N requirement of a week, in the *DetectNitrogen* mode, cannot be determined by the equation [5-3.6] in advance unless the simulation for this week has been finished. This is because the amount of N uptake during a week without N fertilizer, N_{uptake} in the equation [5-3.6], is unknown before the simulation of this week is finished. So MOM first estimates N_{uptake} by simulating this week without N fertilizer applied. Then the amount of N needed during this week, N_{need}, is calculated by equation [5-3.6] and is immediately applied at the end of simulation for the week. Since the applied fertilizer may not be depleted or lost immediately and the crop can usually continue to utilize the fertilizer in following weeks, slightly late (a couple of days) application of N_{need} can be considered as nearly on time when it should be applied at the beginning of the week. The major effects of the applied fertilizer on the soil-plant system will be reflected in the simulation of the following weeks. The simulator repeats the above procedures week by week. At the end of the simulation of *DetectNitrogen* mode, approximate weekly requirements of soil N supply are detected. The results of the *DetectNitrogen* and the *DetectWater* mode are used to generate the primary management combinations (Fig. 5-3.4).

5-3.3.4. Optimization, Predict Growth Modes

After the management combinations are generated, a laboratory is needed to conduct experiments to test these management strategies. The *Optimization* mode is designed as this laboratory. It inputs the dataset as the *Validation* mode does except for the schedule of N fertilizer and irrigation. The *Optimization* mode inputs the data of N fertilizer and irrigation only from the management schedules (combinations) produced by the generator, ignoring the management schedules contained in the dataset if any. Although the *Optimization* mode runs all processes of N-SIMULATOR as the *Validation* mode does, it only outputs three results: crop yields, profits, and leachate nitrate, which are associated with the MOM objectives. The results are saved with the codes of management combinations in a working file called solution.db, which is retrieved by the MOM evaluator later to search for optimal solutions. The few outputs will ensure MOM execution efficiency because the *Optimization* mode will be called repeatedly until optimal solutions are found.

The *PredictGrowth* mode is designed to predict the response of the soil-plant system to the management strategies. Its outputs and inputs are the same as the *Validation* mode's, except for the inputs of N fertilizer and irrigation data that are one of the management strategies that users selected. When an optimal solution is found, users can immediately examine the effects of the solution on the soil-plant system graphically by running the *PredictGrowth* mode. The *PredictGrowth* mode also outputs the simulation results to database files that can be used for further analysis. In addition, the *PredictGrowth* mode is often used to observe the effects of the solutions users selected during the MOM searching sessions. This is an important tool for users to evaluate MOM searches when they try to guide the search process. Users are encouraged to join and guide the MOM searching when they work on specific cases, although the MOM can automatically find optimal solutions. We discuss the reason for this issue in following section.

5-3.4. MOM Evaluator

The evaluator is the "brain" of MOM that uses the built-in knowledge and communication with users to analyze the outputs of the simulator and guide the generator's work. As the specification in section 5-2.1, the evaluator employs artificial intelligence techniques to examine the effects of management strategies to find optimal solutions that produce less nitrate leaching, higher yields and profits.

5-3.4.1. Strategic and Tactical Search

Recalling the terminologies described in section 5-3.1 and Fig. 5-3.1, the evaluator task is to search for the nodes (management combinations) that satisfy MOM goals, among the enormous number of potential nodes. To illustrate the MOM search methods, the management nodes were deployed in two dimensions of MOM sub-goals, potential nitrate leaching versus profits, to form a net for the search (Fig. 5-3.5). The evaluator is assigned to find the nodes that nearly match the two sub-goals: high profits and low nitrate leaching. Note this is an example for discussion. The possible nodes are many more than that the figure displays. The nodes in Fig. 5-3.5 are assumed to be the primary management combinations that are close to the solutions.

Although the search starts near the goals, a limited search time still challenges MOM to exhaust all nodes by simulating a whole cropping season for each node. An effective search algorithm must be developed to find the shortest path from the start node to the goal node without examining all nodes. The *hill-climbing* and *best-first* are two heuristically informed search methods to improve search efficiency (Winston, 1992). The *hill-climbing* search moves through a tree of paths as the *depth-first* search does, except that the choices are ordered according to some heuristic measure of remaining distance to the goal. In the *best-first* search, forward motion is from the best open node so far, no matter where that node is in the partially developed search tree, even though it does not lead to the goal with certainty (Winston, 1992). To ensure MOM reaches the goals effectively, a mixed search method, *hill-climbing* as a

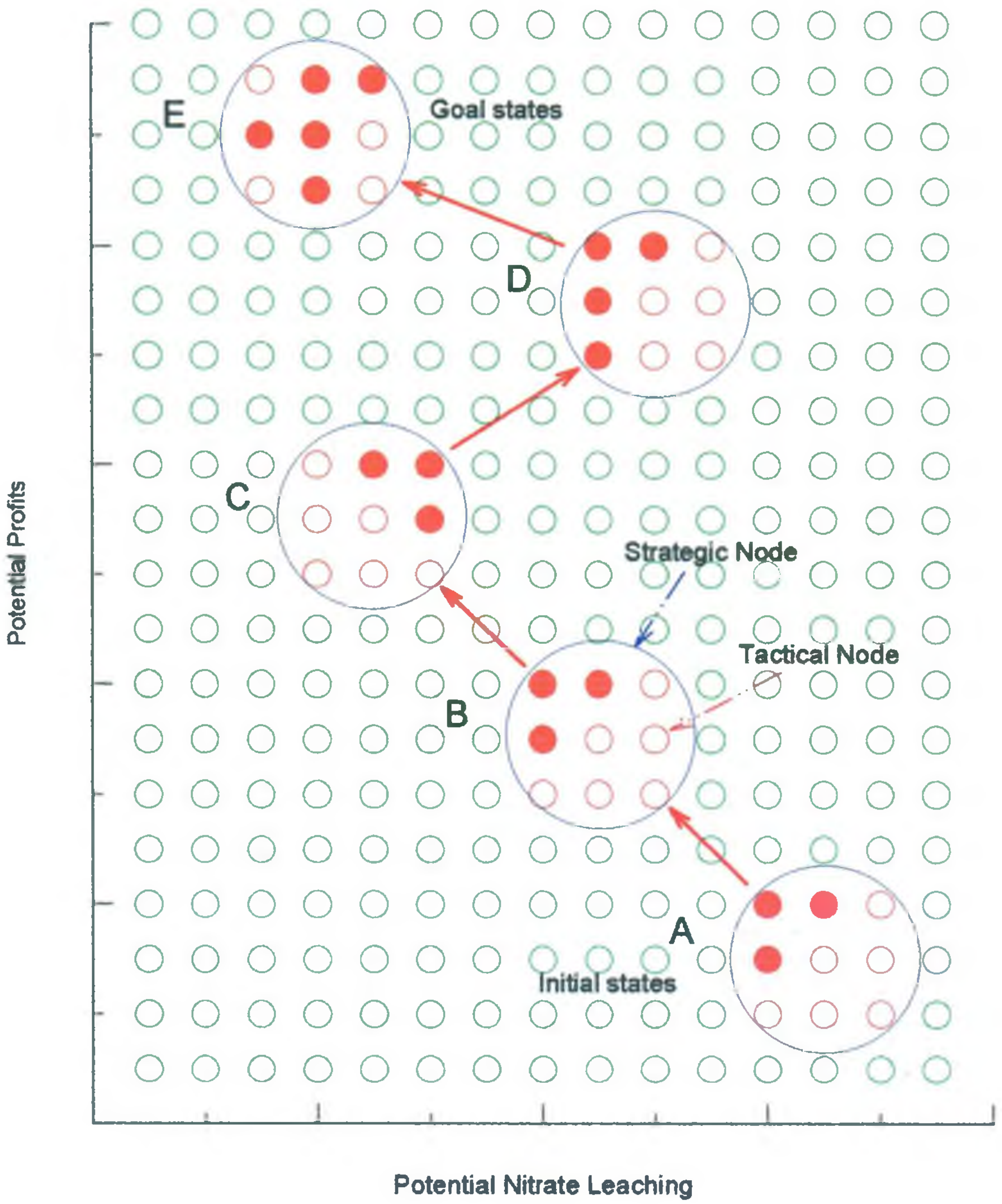

Fig. 5-3.5. A mixed search method with two heuristically informed searches is used in MOM: *hill-climbing* as a strategic search method to find global optimals, *best-first* as a tactical search method to determine local optimals in a strategic search.

strategic search method that embraces *best-first* as a tactical search method [2], was developed for MOM to find the shortest path from start nodes to goals.

The absence of a specific goal state is the second challenge for the MOM search algorithm. MOM cannot specify a certain amount of profit or a specific nitrate leaching rate as a goal before the simulation. In other words, the actual highest profit and the lowest leaching rate are unknown. This problem occurs in other biological systems that employ AI search techniques (Plant and Stone, 1991). However, the heuristically informed search methods require goal information in order to evaluate search paths. So the relative goal state is applied in MOM to measure the relative distances between current nodes and goal nodes. For example, the relative goal state is set as the higher the better for profits while nitrate leaching is always set as low as possible.

Strategic search using the hill-climbing method

The strategic search in MOM is a search among groups of tactical nodes. In the example of Fig. 5-3.5, a strategic search step refers to a strategic node (a big circle marked with "A" or "B" or . . .) that contains nine tactical nodes. So the strategic search is designed to find global optimal solutions among the five big nodes in this example. The search starts from the strategic node "A" that is a group of primary combinations produced by the generator, where profits are not high nor are nitrate

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2 In addition to *hill-climbing* and *best-first* methods, other concepts of AI techniques were involved in constructing the MOM search algorithm. For example, the idea of Means-Ends method (Winston, 1992) was adapted to estimating the distances of current nodes to goal nodes.

leaching estimates low. The tactical search procedure is called to sort this group of nine nodes to determine local optimal nodes, three solid nodes on the upper-left corner. These local optimal nodes indicate that next strategic move should be toward the direction of less nitrate leaching and higher profits. This information [3] is passed to the generator to create new paths by extending the path of the upper-left corner to its neighbors, regardless of the neighbors of the terminal nodes in other directions. These new paths of the second strategic search move, nine nodes within the circle "B," have a shorter distance to the goals than other neighbors of the terminal nodes of the strategic node "A." This *hill-climbing* search calls tactical search procedure again and repeats above processes until the global optimal solutions are found. In this example, the strategic search ends at the strategic node "E," where there is no clear path information that leads to a better solution than current state. The solid nodes within the circle "E" are global optimal solutions that have relative high profits and lower nitrate leaching potentials than others for this example. Users can choose one of these solutions that is suitable to their particular situation to schedule the N management. *Hill-climbing* considerably improved the search efficiency in this example by examining only 45 nodes among a total of 300 nodes. A scenario of the *hill-climbing* strategic search is shown in Fig. 5-3.6, in which the dataset of the summer corn (See section 4-5.3) is used with hypothetical economic data. In the scenario, there are five strategic nodes and each strategic node contains 36 tactical nodes that will be discussed in the following

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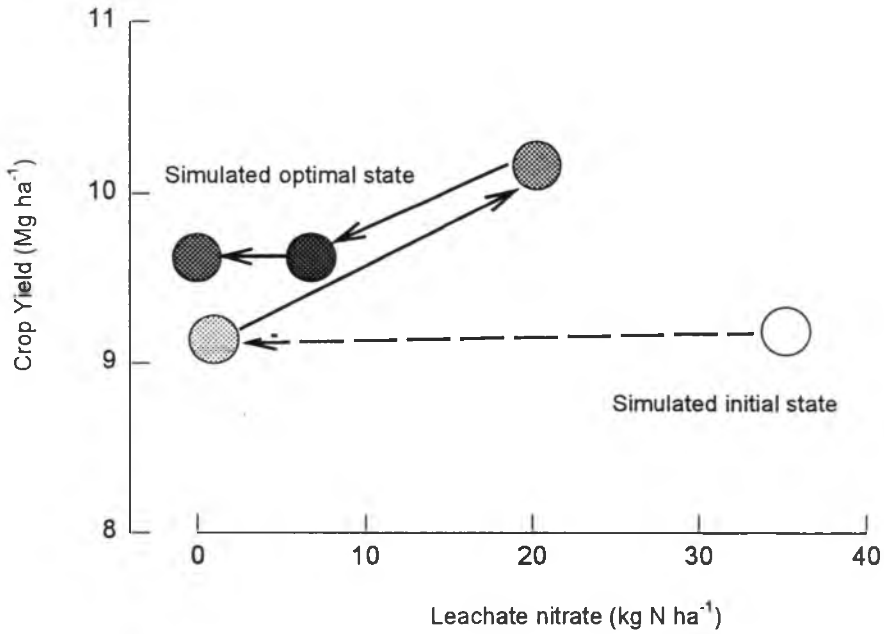
[3] Path information indicates whether to increase or decrease the rates of the fertilizer and irrigation. Detailed discussion is in following paragraph.



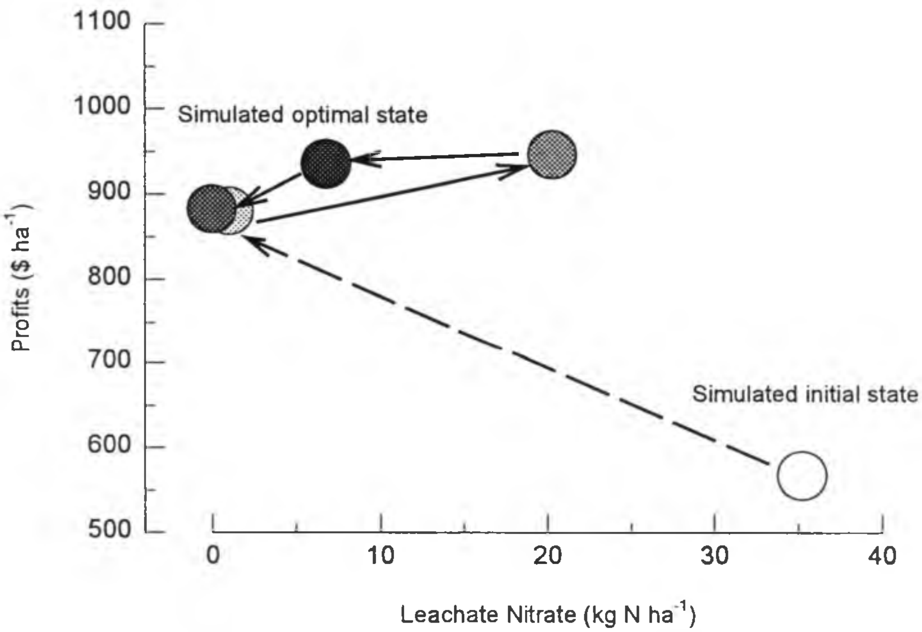


Fig. 5-3.6. A scenario of the *hill-climbing* strategic searching in MOM. The search leads to higher profits, yields and less nitrate leaching. The dataset of the summer corn (section 4-3.4.3) is used in the scenario with hypothetical economic data.

paragraph. The strategic search paths in Fig. 5-3.6 illustrate that MOM would have improved management strategies, which would have increased profits and reduced nitrate leaching.

Tactical search using the best-first method

A tactical search in MOM is a search to find local optimal choices among the nodes within a strategic search move. In the example of Fig. 5-3.5, tactical search means to find the nodes whose states are closer to the goal states than others among nine nodes within a strategic node (e.g., in a circle "A" or "B," or others). The *best-first* search is applied as the tactical search method because the paths found by this method are likely to be shorter than those found with other methods (Winston, 1992). In the *best-first* search, MOM orders the tactical nodes by their states. The node which state is the closest to the goal state goes first, the closer second, and the node whose state is far away from the goal is the last to be selected (how to measure a node's state will be discussed in the section 5-3.4.2). Then MOM examines the first 3 - 5 nodes to determine the path information for the next strategic move by comparing the states of nodes. The path information in MOM consists of five management factors: fertilizer rate, frequency, irrigation rate, frequency, and fertilizer in irrigation. MOM analyzes the first 3 - 5 nodes in the search queue by below rules:

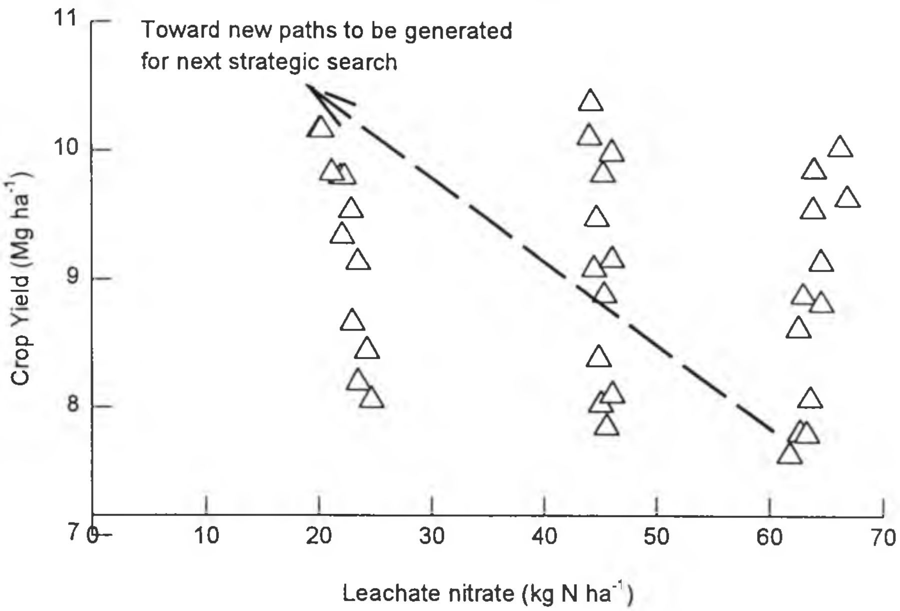
1. IF a level of a factor (e.g., a fertilizer rate) is shared by these nodes, THEN the next strategic search for this factor should move toward the direction that this level indicates.
    1.1. IF the shared level is at the end of the highest level, THEN the level of the factor should increase in the next strategic search.

1.2. IF the shared level is at the end of the lowest level, THEN the level of the factor should decrease in the next strategic search.

1.3. IF the shared level is in between both ends, THEN the level of the factor should not change in the next strategic search.

2. IF no levels of any factors are shared by these nodes, THEN a plateau state is reached. The automatic strategic search pauses and waits for instructions from the user.

If the first three nodes (solid nodes) in the strategic node "B" share the highest level of the fertilizer rate, for example, the fertilizer rate will be increased in generating the next group of management combinations (the strategic node "C"). The plateau state found by the automatic strategic searching is often near the goal state even though it may be a local optimal state in some cases. If the nearly-optimal solutions satisfy the user's requirements, the solutions can be considered as global optimal solutions. However, the user can continue to search until a better state is found. An example of the *best-first* tactical search is illustrated in Fig. 5-3.7, in which 36 tactical nodes are contained in a strategic node that is shown in the scenario of Fig. 5-3.6. The arrows across the diagrams indicate the direction of the next strategic move: increase profits and yields while decreasing nitrate leaching. The arrows also indicate the ordering of the nodes that are sorted by *best-first* search. The first couple of paths in the search queue (whose distances to the goals are shorter than all others) appear in the upper-left corner in the diagrams. The last paths that are far away from the goals sit near the low-right corner in the diagrams.



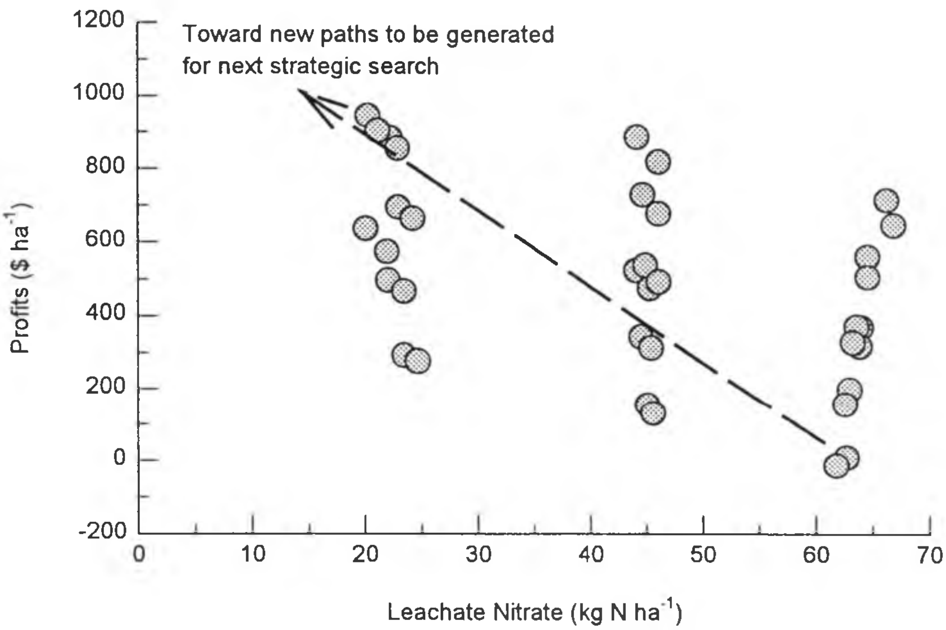


Fig. 5-3.7. A scenario of the *best-first* tactical searching within a strategic search. The dataset of the summer corn (section 4-3.4.3) is used in the scenario with hypothetical economic data.

5-3.4.2. Goal Weighting and Search Direction

To sort current tactical nodes in the *best-first* ordering, a measurement is needed to determine the distance from the current node's state to the goal node's state. The state of each node is represented by its three characteristics in MOM: profit, yield and leachate nitrate. The measurement of each single state characteristic can be usually estimated by the difference between a current state and the goal state. But this distance cannot be measured in MOM because the goal state of MOM is not a specific state as the discussion in section 5-3.4.1. Therefore, a **relative distance**, D_i, was developed as a measurement to order the tactical nodes in MOM, though the absolute distance is unknown.

$$D_i = (X_{Goal} - X_{Min}) / (X_i - X_{Min}) - 1.0 \qquad [5\text{-}3.7]$$

where $X_{Goal} \geq X_i \geq X_{Min}$. X_{Goal} refers to the goal state variable that can be a local goal or a global goal. X_{Min} represents the state variable with minimum value among a group of tactical nodes in one strategic node, or the minimum in global. X_i is the state variable representing the current value of a state characteristic of the node i. The D_i value represents a relative distance from the node i to the goal. The equation [5-3.7] is applied in MOM for sub-goals of profits and crop yield. It is interpreted as the higher the state variable value, the shorter the distance to the goal. When $X_i = X_{Min}$, $D_i \rightarrow \infty$. When $X_i = X_{Goal}$, $D_i = 0$, the goal is reached. For the sub-goal of minimizing nitrate leaching (the less the leaching, the shorter the distance to the goal). Its $D_{leaching,\,i}$ is calculated by

$$D_{leaching,\,i} = (X_{Max} - X_{Goal}) / (X_{Max} - X_i) - 1.0 \qquad [5\text{-}3.8]$$

where $X_{Goal} \preceq X_i \preceq X_{Max}$. X_{Max} is the state variable with maximum value among a group of tactical nodes in one strategic node, or the maximum in global. It represents the maximum nitrate leaching rate at local conditions. X_{Goal} is the goal state variable that can be a local goal or a global goal. The minimum goal is no nitrate leaching, $X_{Goal} = 0$. X_i and D_i refer to the same meanings as those in the equation [5-3.7]. The equation [5-3.8] is interpreted as the smaller the state variable value, the shorter the distance to the goal. When $X_i = X_{Max}$, $D_i \rightarrow \infty$. When $X_i = X_{Goal}$, $D_i = 0$, the goal is reached.

Another challenge of the MOM search is that three state characteristics (sub-goals) must be considered simultaneously even though sometimes three sub-goals may conflict with each other. For this challenge, a linear weighting method is developed to integrate three characteristics into one measurement, a **relative weighted distance**, to estimate the space difference from a current node to the goal state. The relative weighted distance of node i, $D_{wt,\,i}$, is expressed as

$$D_{wt,i} = \frac{1}{\left(W_p \frac{X_p - X_{Min}}{X_{Goal} - X_{Min}} + W_y \frac{X_y - X_{Min}}{X_{Goal} - X_{Min}} + W_l \frac{X_{Max} - X_l}{X_{Max} - X_{Goal}}\right)} - 1.0 \qquad [5\text{-}3.9]$$

where X_{Goal}, X_{Max} and X_{Min} refer to the same meanings as those in the equation [5-3.7] and equation [5-3.8] respectively. X_p, X_y, and X_l represent current state variables of the profit, crop yield, and leachate nitrate respectively, as X_i in the equation [5-3.7] and equation [5-3.8]. W_p, W_y and W_l refer to the weights of the profit, yield, and nitrate leaching in estimating the distances to the goal. The values of weights depend on users' objectives and are unified by

$$W_p = W_p / (W_p + W_y + W_l) \qquad [5\text{-}3.10a]$$

$$W_y = W_y / (W_p + W_y + W_l) \qquad [5\text{-}3.10b]$$

$$W_l = W_l / (W_p + W_y + W_l) \qquad [5\text{-}3.10c]$$

Finally the **relative weighted distance,** D_{wt}, can be used to estimate the shortest path directing to the next strategic search. Using the *best-first* search procedure, MOM sorts out tactical nodes within a strategic search step into a queue in ascending order by their D_{wt} values. The usage of this queue for the tactical search was discussed in the last section 5-3.4.1.

The goal weights are used to direct the searching. If the weights of three goals are changed, the relative distances, D_{wt}, are changed (equation 5-3.8). And the order of tactical nodes in a search queue is changed. Finally the direction of the next strategic move is changed. So the goal weighting is an important tool for users to guide MOM's search. An example of differing goal weights in the scenario (used in section 5-3.4.1) illustrates that the goal weighting changes the first five tactical nodes in a search queue and also changes the final choice of optimal solutions (Table 5-3.2).

Table 5-3.2. The first five tactical nodes in the queue of the final strategic search are changed by differing goal weights.

Goal wt-1	50%	50%	50%	Goal wt -2	65%	50%	35%
Node #	Profit $\$\ ha^{-1}$	Yield $kg\ ha^{-1}$	Leaching $kg\ N\ ha^{-1}$	Node #	Profit $\$\ ha^{-1}$	Yield $kg\ ha^{-1}$	Leaching $kg\ N\ ha^{-1}$
#35	880	9138	0	#34	935	9621	6.8
#29	855	9138	0	#35	880	9138	0
#23	831	9138	0	#31	904	9520	5.5
#34	935	9621	6.8	#28	911	9621	6.9
#31	904	9520	5.5	#29	855	9138	0

With Goal wt-1 in Table 5-3.2, the first solution choice is Node# 35 with profit \$880 and no nitrate leaching, which management combination consists of 154 kg N ha^{-1} N fertilizer applied in two weeks and 229 mm irrigation in 14 weeks during the 15-week cropping season. However, if the search is controlled by Goal wt-2 which weights profit higher than nitrate leaching, the first five nodes in the queue and their orders are changed. The first solution choice is changed to Node# 34 with profit \$935 and 6.8 kg N ha^{-1} nitrate leaching, which management combination consists of 154 kg N ha^{-1} N fertilizer applied in two weeks, and 274 mm irrigation in 14 weeks during the cropping season.

5-3.4.3. Interaction to Guide Search

MOM is designed as a **decision-aid** to assist users in finding a solution that meets their goals, not a tool that makes decision for users. As discussed above, MOM's "intelligence" consists of very limited equations and rules. It will lose its way if problems are not covered by the equations and rules. For example, *hill-climbing* method has some problems in searching such as "foothills, plateaus, and ridges" that are hard to "climb" (Winston, 1992). To avoid making mistakes, the MOM search style is designed to accept user interaction. It implements the strategic search under the user's guidance plus an automatic search procedure that works well in most situations. However, if the search reaches a plateau, users must determine how to change the management combinations (five factors discussed in section 5-3.4.1) for the next strategic search move, or declare that the goals are reached. The goal weights that represent the users' objectives can be used to control either the global search or the tactical search. To assist user analysis of the search processes, MOM provides users with on-line state space diagrams (Fig. 5-3.8) as graphic tools that examine the search. Users can determine the current relative weighted distances of any nodes to the goal immediately, just using the mouse to circle the nodes on the state space diagrams (Fig. 5-3.8). A user with N management knowledge can adjust the management factors manually between strategic search moves.

In addition to guiding the search, users must make the final decision in choosing optimal solutions from the final solution list. This is because an optimal solution may not necessarily fit a user's particular situation. Therefore, the MOM interface is designed to facilitate the search sequence as well as to list alternative solutions for users' choices.

5-3.5. MOM Execution

As a summary of the MOM implementation, a MOM session is briefly described in this section and in Fig. 5-3.9. A MOM session proceeds as follows:1.

Detect the shortages of soil N and water for a cropping season. This results in a primary management combination (an N fertilizer and irrigation schedule) that is close to matching crop requirements.

2. Start a strategic search.

   2.1. Assemble a group of new tactical search nodes using the generator. The tactical nodes consist of the combinations of management factors: N fertilizer rate and timing, irrigation rate and timing, and fertilization with irrigation systems. The adjustment of the factors would bracket the

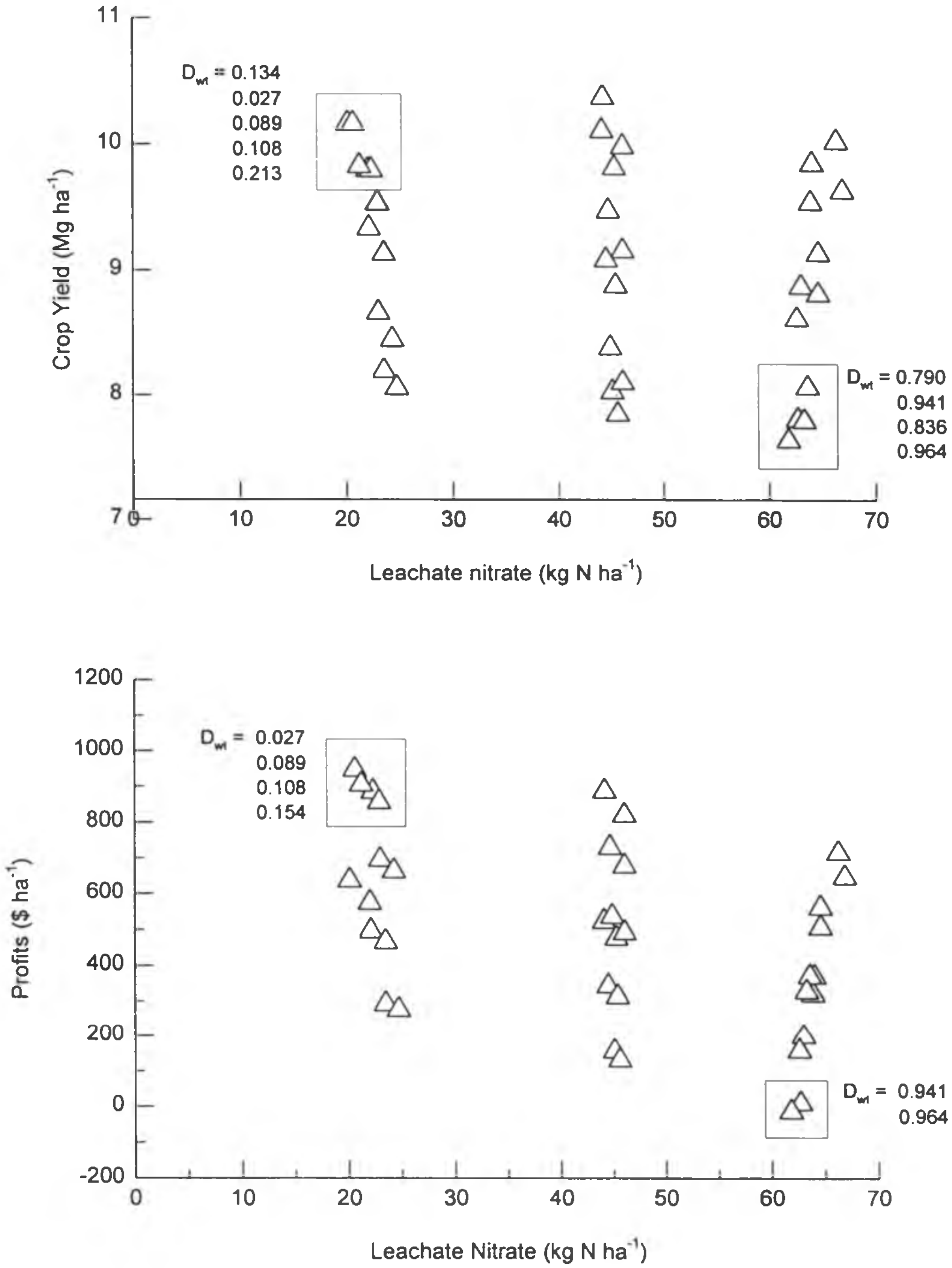


Fig. 5-3.8. Examples of the state space diagrams for on-line search analyses. The relative weighted distances from current nodes to the goal, D_{wt}, are displayed if they are selected by the mouse.

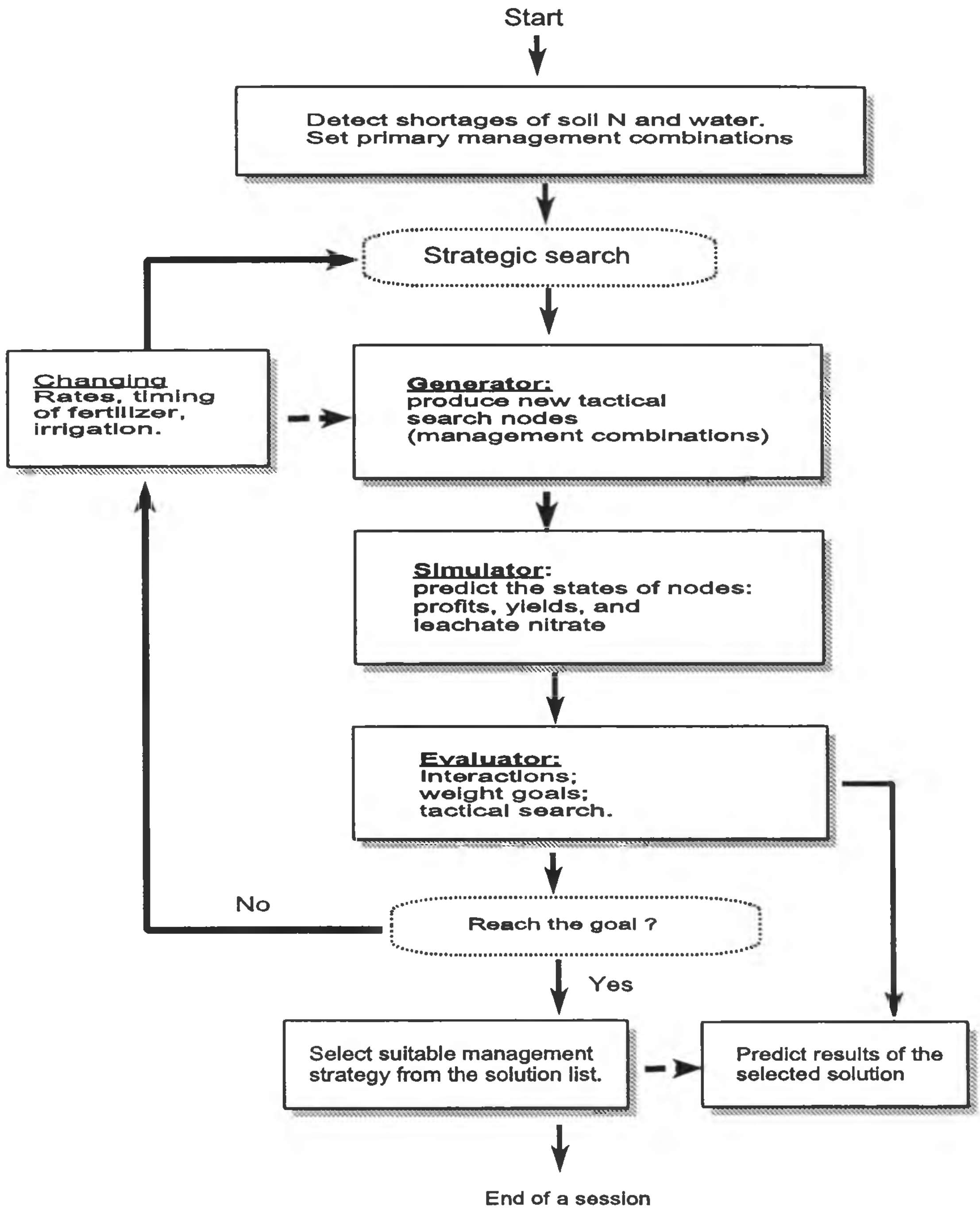


Fig. 5-3.9. Flow chart of MOM implementation

primary management combinations at the first strategic search and bracket the last combinations at following strategic searches.

2.2. Predict the states of current tactical nodes using the simulator. The node's state in MOM consists of three characteristics: the profit, yield, and nitrate leaching. The characteristics of the goal state are also called sub-goals.

2.3. Assess the states of current tactical nodes using the evaluator. (1) Adjust the weights of three sub-goals. (2) Estimate the relative weighted distances between current nodes and the goal. (3) Search tactical nodes to find the shortest path toward the goal.

3. Determine if a plateau has been reached.

3.1. If a plateau is not reached, the path information resulting from the tactical search is transferred to the generator to create a new group of tactical nodes by extending the desired neighbors of the terminal nodes. Then repeat step 2.

3.2. If a plateau is attained, users must judge whether the plateau is a local or global optimal situation [4].

3.2.1. If the plateau is a local optimal, change the management combinations manually and repeat step 2.

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[4] It is an optimal situation among situations produced by all management choices in a global search.

3.2.2. If the plateau is the global optimal, the goals are reached and the search succeeds. Select suitable solutions from the solution list for displaying results.

4. Graphically demonstrate the predicted effects of selected management combination on the soil-plant system, during the search or at the end of the search.

5-4. Summary

Dramatically increasing nitrate pollution in groundwater in recent years requires that we learn to control N pollution by finding optimal management strategies to reduce the contamination. Among optimization techniques in agriculture, a hybrid simulation model and knowledge-based system developed in recent years, is a useful approach to solve the nitrate leaching problems in dynamic soil-plant systems. However, existing N models were not designed with AI optimization for dynamic precision N management. Management-Oriented Modeling (MOM), a dynamic simulation modeling with artificial intelligence (AI) optimization techniques, has been developed in this study to provide a precision tool in finding optimal solutions for N management to minimize nitrate leaching and maximize production and profits.

MOM consists of a generator, a simulator, and an evaluator. In searching optimal management strategies, the generator produces a group of nodes (management choices). The simulator predicts the results of the nodes such as nitrate leaching, production and profits. The evaluator is the core of MOM that uses the built-in knowledge and communication with users to analyze the outputs of the simulator and guide the generator's work. To ensure MOM reaches the goals effectively, a mixed search method, *hill-climbing* as a strategic search method that embraces *best-first* as a tactical search method, was developed to find the shortest path from start nodes to goals. Examining the tactical nodes in a strategic search, the evaluator finds short paths toward nearly optimal solutions and passes the path information to the generator. The generator uses the information to produce the next group of tactical search nodes that are closer to the global optimal solutions.

MOM is a goal-driven modeling system in which the simulation is directed toward user-weighted goals. The model can be used as a tactical N management tool for in-season management of specific conditions and used as a strategic N management tool for general decision rules. MOM was also constructed as a tool for diverse users from farmers to scientists. MOM can usually find the nearly optimal solutions in 5 - 20 minutes on current personal computers. In a maize production scenario, MOM found a nearly optimal management solution that would have increased the profit from \$570 to \$935 ha^{-1} and reduced the nitrate leaching from 36 to 7 kg N ha^{-1}. The results show MOM is a useful modeling method for dynamic N management.

Chapter 6

MOM-guided Within-season Management

In-season management decision aids are very important to nitrogen management because the final fate of the N in soil-plant systems largely depends on the in-season management. Nitrogen is the plant nutrient that is applied in the largest quantity in fields for production. Inorganic N (mostly in nitrate or ammonium form) is highly water-soluble in soil-plant systems. The status of inorganic N in soils rapidly changes with crop growth and management practices during a cropping season. In upland field conditions, almost all ammonium was converted to nitrate in one month (Khan, *et al.*, 1986). Nitrate is highly mobile in most soils and can easily move below the root zone, where nitrate becomes inaccessible to crops and is subject to leaching into groundwater. In high leaching risk areas with sandy soils or heavy rainfall, N fate is very sensitive to rainfall events, the rates and timing of N fertilization and irrigation. Theoretically, N management strategies can be well scheduled and planned off-season based on historical weather data, in which the N fertilizer supply can be synchronized with the plant needs. However, the uncertainty of rainfall results in sub-optimal management if based on a fixed schedule. For example, if unexpected heavy rain falls during or just after a large application of N fertilization, a significant amount of N fertilizer intended for crop uptake may be leached beyond the root zone. The N fertilizer intended for crop growth then becomes a potential N pollutant, which imposes two impacts on the soil-plant system. One is a shortage in N supply for crop growth and another is the risk of damaging the environment. Facing this kind of in-season change, the management schedule should be flexible for within-season adjustment to avoid serious leaching events while supplying sufficient N for crop growth.

When a nitrogen model is used to guide within-season N management, it must deal with the uncertainty of coming weather. Stochastic models are usually designed to estimate spatial and temporal uncertainties in prediction. However, so far stochastic models of soil-plant systems are difficult to apply to field management (Ling, 1996). Another method for in-season management is real time control. Sensor technologies and soil tests are being developed to provide feedback of soil-plant systems for adjusting management practices.

MOM is not a stochastic model, but a two-way modeling model that simulates natural processes and human management practices (See section 5-2.2). So MOM is designed as a within-season tool for nitrogen management as well as a tool for research, teaching, planning, assessment, and general management. Within a cropping season, MOM recommends adjustments in the management to fit current weather conditions and the changes of soil-plant systems. This two-way modeling style works as a modeled real time control system for within-season management. Because MOM focuses on assisting N management **within a real cropping season,** this MOM working mode is called **MOM-guided within-season management**, differing from the models for general management. This chapter first examines weather generator models and monitoring with soil tests or sensors for N in-season management. Then the concept and implementation of MOM for within-season management are discussed to illustrate how MOM attempts to dynamically optimize N management within a cropping season.

6-1. Weather Generator Models

For many agricultural models, one of the greatest uncertainties is future weather. To deal with this unknown, a stochastic module called a weather generator is usually added to system. An example of this type of weather generator, WGEN, was developed by Richardson and Wright (1984). WGEN works as a random weather generator that produces daily maximum and minimum temperature, rainfall, and solar radiation based on longitude and latitude for the cotton-heliothis hybrid systems discussed in section 5-1. Another weather simulation model is "NATCOVER," which was developed to improve the accuracy of crop simulation models (Wang and Whisler, 1996). Constructed from historical daily weather data for the GOSSYM/COMAX cotton simulation model, "NATCOVER" generates several weather patterns based on long-term climatic data under normal conditions, and with six other hypothetical weather scenarios.

Weather generators are useful for agricultural models in general applications in research, teaching, planning, and assessment. If models are used for in-season applications, weather generators still face challenges. Stone and Schaub (1990) compared the weather data generated by WGEN with measured field data and historical averages. Patterns of the generated data looked much like actual field data. However, the generated data were less likely to match field conditions than the average data on any particular day. Although the averages provide better estimates on given days, Plant and Stone (1991) concluded that the average season is not a realistic approximation of a particular season's weather. There is no such as a thing as a "typical year."

6-2. Soil Test and Sensor Monitoring

Binford *et al.* (1996) proposed in-season soil testing for monitoring nitrogen management based on sugar beets experiments. In the experiments during 1993, 1994, and 1995 seasons in western Nebraska and Wyoming, ten rates of N (0 to 304 kg N ha^{-1} in 34 kg N ha^{-1} increments) were applied in four replications before planting. Soil samples, 0-30 cm, were collected at two-week intervals and analyzed for nitrate concentration. They found that net returns to N fertilization decreased significantly as the soil nitrate concentration increased to 40 mg N kg^{-1}. On-site soil nitrate testing as a method of monitoring N fertilizer management was also suggested by Marx *et al.* (1996). The on-site monitoring practice was called the Pre-sidedress Soil Nitrate Test

(PSNT). Nitrate was extracted from 10 ml of field-moisture soil, measured by displacement, and analyzed using a quick-test field kit (Nitrachek ™). The field test results were adjusted for difference caused by soil texture and moisture, based on correction factors calibrated from standard laboratory methods.

Another technology used in nitrogen in-season management is real-time control using sensors. To monitor crop N status, Schepers *et al.* (1996) mounted nitrogen sensors on a high-clearance sprayer and interfaced with the spray control system of the equipment. The sensor readings from the adequately fertilized strip were compared with those from adjacent strips that were likely to develop N stress. If needed, N fertilizer was applied to field strips in the spring. Blackmer and White (1996) reported using remote sensing to identify spatial patterns of nitrogen fertilization. Sensor technologies have been successfully applied in many agricultural fields, including monitoring N fertilization for some crops based on tissue N deficiency. N sensors monitor crop N status by detecting its color. Sensors can only determine crop N requirements when it can detect the symptom of a crop N stress. For many crops, however, N fertilizer should be applied a couple days or weeks in advance of when a crop needs N or the crop shows N stress. In other words, the sensor's recommendation for N fertilizer is usually too late to be effective in meeting the N demand of these crops. This situation occurred in most experiments reported by Schepers *et al.* (1996).

6-3. Using MOM to Guide Within-season Management

Considering the capability of MOM in predicting N status in soil-plant systems at acceptable accuracy (See section 4-5), MOM was also developed for within-season simulations to optimize nitrogen management, called MOM-guided within-season management.

To make decisions for within-season N management without a decision-aid, a decision-maker usually first collects the necessary data that include current crop N status, soil N and moisture status, and precipitation (Fig. 6-3.1). The data can be collected from soil tests, sensors, and weather forecasts. Then the decision-maker analyzes the data and estimates the amounts and timing of N fertilizer and irrigation in the following weeks.

If MOM is calibrated and validated to local conditions, it can simulate the above decision-making process without within-season data from soil tests or sensors, except for initial site conditions. Fig. 6-3.2. illustrates the concept that MOM navigates within-season N management by mimicking the process above. Primary purposes of MOM-guided within-season N management are: (1) Use simulated data to substitute for within-season soil and tissue test data. (2) Use the model to dynamically monitor and navigate within-season N fertilization and irrigation. Assume MOM was calibrated and validated to a specific site and a decision-maker had made initial soil tests for soil N and moisture just before planting. A MOM-guided within-season N management is described below (Fig. 6-3.2).

1. Run MOM before planting to schedule seasonal management strategies, based

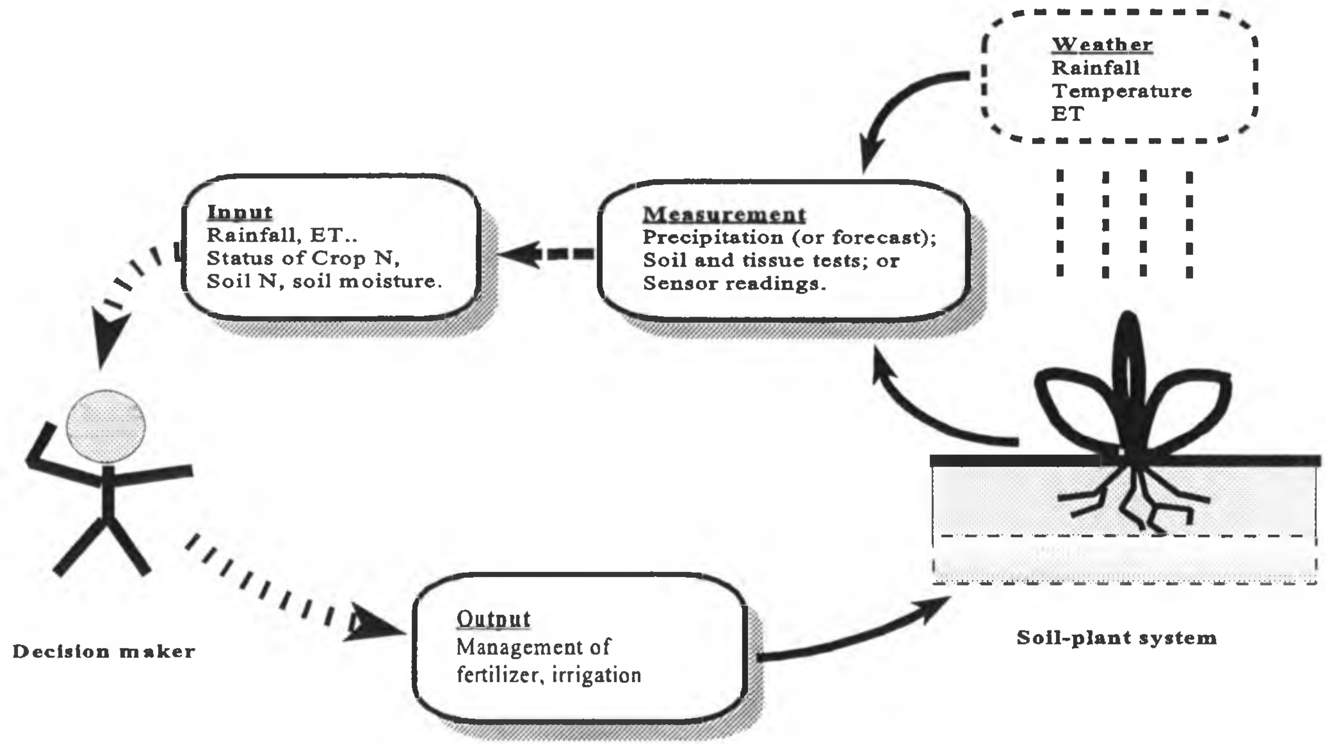


Fig. 6-3.1. A diagram of within-season N management without decision-aid. Current information of the soil-plant system is collected from soil tests, sensors, and weather forecasts. A decision-maker analyzes data and estimates the amounts and timing of N fertilizer and irrigation in following weeks.

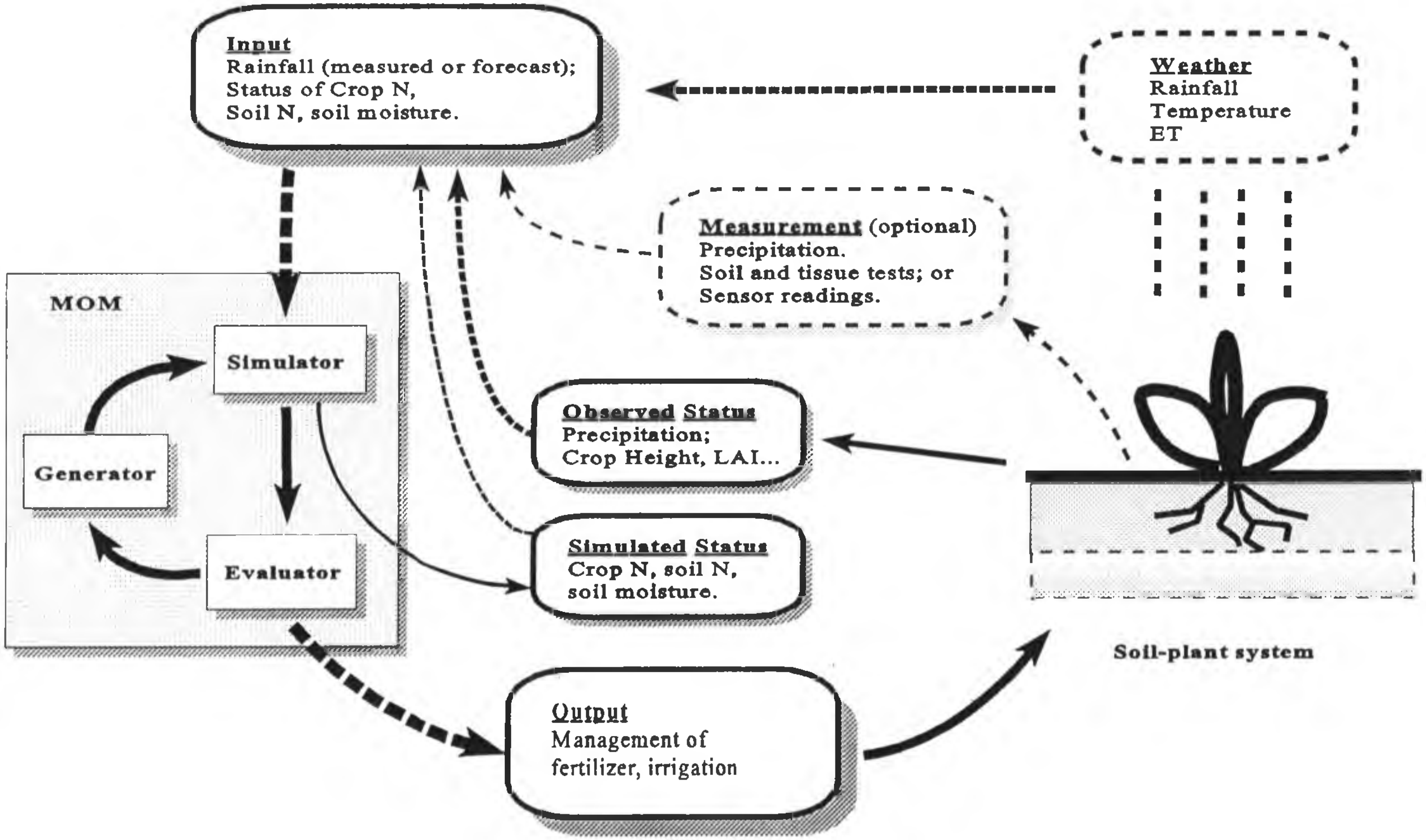


Fig. 6-3.2. A diagram of MOM-guided within-season N management. Current information of the soil-plant system comes from simulated data and weather forecasts. MOM's evaluator analyzes data and optimizes the management schedule for the following weeks.

on initial conditions of the soil-plant system and weather data from historic averages (or from weather generators if users have). MOM simulates the N cycle of the entire cropping season and predicts possible optimal crop yields, profits, leached nitrate, and other outputs, as well as corresponding management strategies of N fertilizer and irrigation.

2. Run MOM weekly (or shorter intervals if necessary) to update and monitor the current status of the soil-plant system.

    2.1 Input actual precipitation, irrigation, and N fertilization of the past weeks to update current status of N and water in the soil-plant system of the model. MOM displays the simulated status of the soil-plant system before TODAY in solid lines (Fig. 6-3.3).

    2.2 Input the forecast amounts of precipitation in following weeks if they are significantly different from those in MOM databases. Then MOM **re-simulates** and updates the status of the soil-plant system after TODAY, shown in dotted lines (Fig. 6-3.3). MOM also **reevaluates** the management strategies after TODAY and **updates** the management schedule for the following weeks.

3. Rainfall is uncertain for within-season management but is important to simulate N movement in soils. Weekly observed precipitation inputs are necessary for MOM-guided within-season management. Updating weekly air temperature and ET is not required by MOM unless the season climate changes fundamentally. Some simple functions of crop uptake N related to the crop

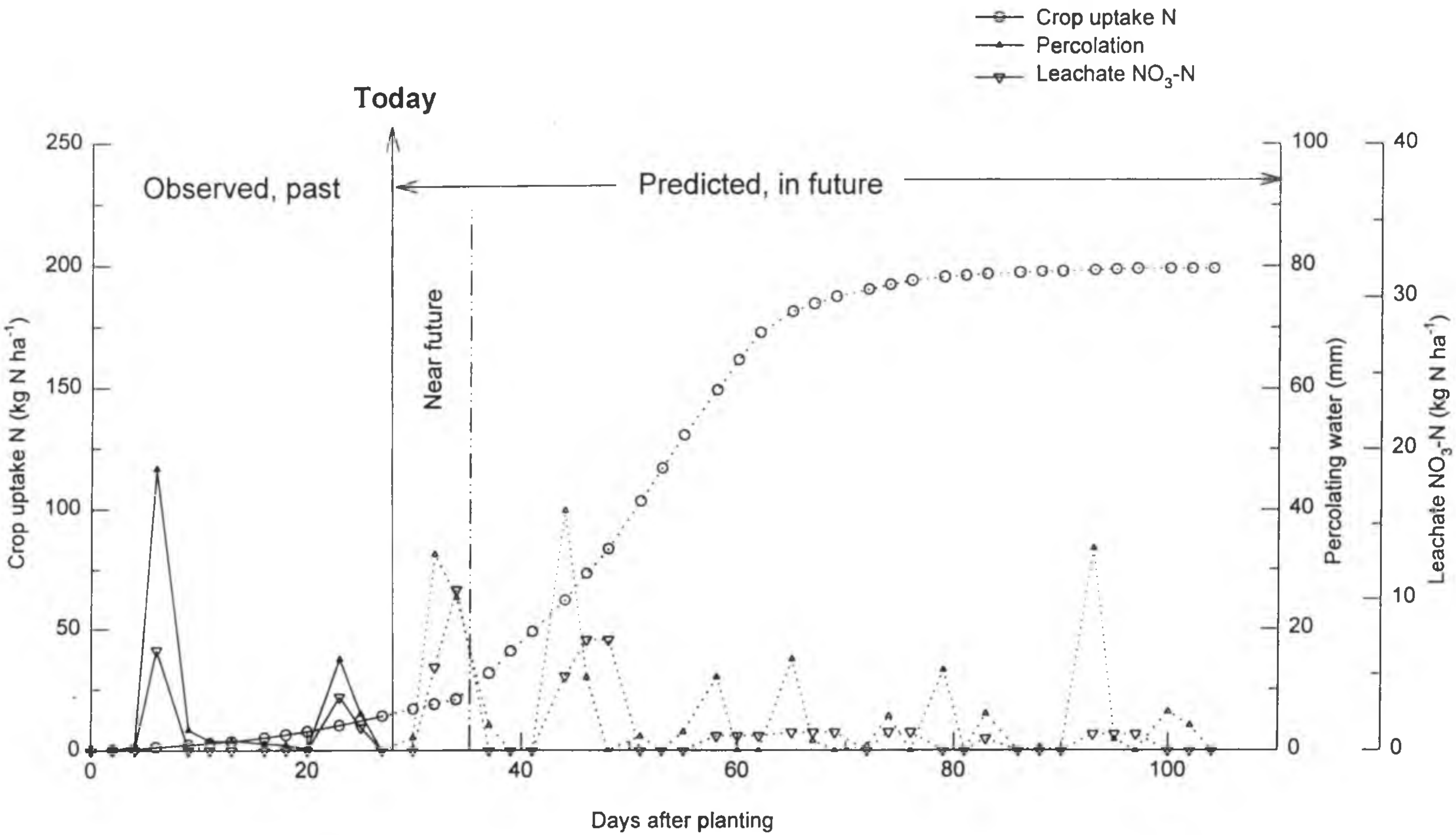


Fig. 6-3.3. MOM-guided within-season management shows status of the soil-plant system before TODAY in solid lines, status after TODAY in dot lines. MOM can do nothing for the past but can change the management schedule to avoid coming leaching peak in near future (30~35 days after planting).

growth observations, such as $N_{uptake} = f\,(LAI,\ Height_{crop})$, can be established by users. These functions can be used to update growth curve of the crop demand N by easily observed data. The update is helpful when the crop grows abnormally due to unpredicted events such as serious pests. In season soil test data are also helpful in tracing soil N status, but not required because MOM uses its simulated data to monitor the N status of the soil-plant system (Fig. 6-3.2). If MOM was calibrated and validated to a specific site, the accuracy of the simulated soil data may not be less than those of limited field sample tests (Refer to section 4-5, N-SIMULATOR verification/validation).

4. MOM-guided within-season management can run in many ways:
    4.1. On-site or on-field. Users run MOM for a specific crop in a field. A single MOM database is needed for a cropping season.
    4.2. On-farm or on-watershed. Multiple MOM databases are needed for diverse crops and soils in an area. Farmers, watershed managers, extension agents, and consultants may wish to use MOM this way.
    4.3. Soil test reports with MOM. If a sample analysis requires recommendations for N fertilization, MOM may be useful for consultants in (1) demonstrating the N situations of clients' soil-plant systems, (2) optimizing the recommendations for within-season management and (3) illustrating the effects of recommendations on the soil-plant systems in advance.

Within-season management using MOM is a dynamic optimization process. MOM always optimizes the management schedules at weekly or shorter intervals, based on within-season monitoring and updating of the status of the soil-plant system. A perfect optimal management schedule for the whole cropping season may not be guaranteed by MOM-guided within-season management, because of many uncertainties beyond the control of either decision-makers or models. PAST events cannot be revised before TODAY. However, MOM-guided within-season management can improve management in the near future (e.g., the following week) after TODAY. For example, nitrate leaching events occurred in 5-7 days and 22-26 days after planting in Fig. 6-3.3, no matter whether these were failures of the rain forecasts or other reasons. MOM just simulates the past situation and focuses on changing the management schedule after TODAY to avoid the coming leaching peak in the near future (30-35 days after planting). In other words, MOM can help the decision-maker reduce the possible coming leaching peak by trying alterative schedules of fertilization and irrigation. MOM uses a weather forecast to predict effects of coming water events on the N cycle in soil-plant systems. This in turn allows MOM to search new management schedules to update recommendations that adjust for the coming effects. MOM may not perfectly control all events during the whole cropping season but it dynamically traces crop requirements and updates fertilization and irrigation schedules to fit changing weather in the near future. In comparison of Fig. 6-3.3 (status of 28 days after planting) with Fig. 6-3.4 (status of 91 days after planting), MOM did not exactly predict the patterns of water events and nitrate leaching between 28 and 91 days after planting. However, MOM reduced nitrate leaching by updating management of irrigation and fertilization

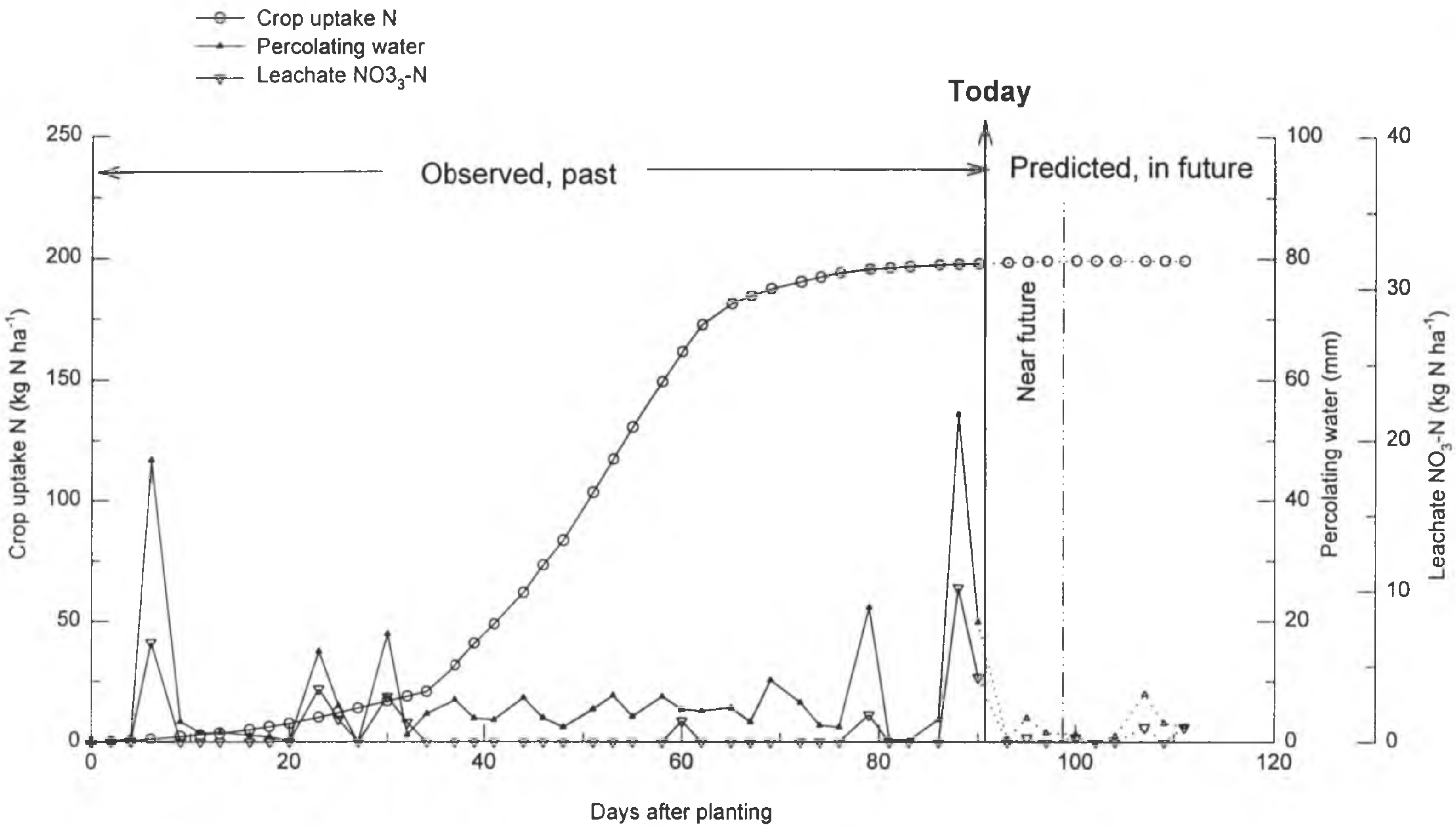


Fig. 6-3.4. MOM-guided within-season management may not perfectly update the schedule to fit uncertainty of rainfall. It improved management in near future. Comparing Fig. 6-3.3 with Fig. 6-3.4, MOM traced crop N requirement and avoided most leaching events.

during the period. This situation illustrates the key **purpose of MOM-guided within-season management**: *not intending to match future events exactly, but updating the model systems within-season and dynamically adjusting management strategies to fit changing conditions*. In addition to its management-oriented optimization, using MOM-guided within-season management has the advantages of:

(1) **High efficiency**. Users can know the probable status of soil-plant systems in a few seconds, without waiting for the results of sample tests. MOM-guided within-season management advises when and how much N that crop demands in advance of sensors and soil tests.

(2) **Low cost**. There is no cost of the N sensors' hardware, and no within-season soil or tissue sampling and testing other than an initial soil test.

(3) "**Transparency**." Daily pictures of the simulated N cycle in soil-plant systems graphically show users predictions of where their N fertilizers would have been, where will be, and how to control them. MOM also presents estimates of N fate in soil-plant systems such as leachate nitrate and mineralized N, which are not provided by standard soil tests.

A major limitation of MOM-guided within-season management is that all simulation results are based on the assumption that MOM is correctly calibrated and validated to specific sites and crops. However, the discussion above illustrates that MOM-guided within-season management is promising for precision N management.

6-4. Scenarios of MOM Optimized Management

MOM validation should include two parts: simulation of natural processes and simulation of management activities, because MOM was designed as a two-way modeling tool (See section 5-2.2). Validation of MOM with respect to the natural processes is to compare the agreement (or closeness) of the model predictions with the observations. This is a validation of the MOM simulator, N-SIMULATOR, which was initially evaluated in section 4-5. The validation of management activities is to compare the differences between the results of existing management practices produced with those that MOM suggests. It is to test whether MOM improved the existing management strategies or not, and the degree of the improvement. This validation requires datasets that consist of, at least, two types of observed data: results produced under existing management practices and results produced under MOM-guided management. In addition to analytical data of soil-plant systems, the dataset should include profits, yields and leachate nitrate, which are three sub-goals of MOM. Unfortunately no such dataset was available when MOM was initially developed. However, an approximate test of MOM predictions for N management can be obtained by testing its simulator as in section 4-5. Several examples of MOM applications to optimize nitrogen management are discussed through scenarios in this chapter. The discussion focuses on how MOM adjusts N management to fit changing conditions during a cropping season. The detail processes are available in the Appendix B.

Five scenarios of MOM-guided N management for upland crops in the tropics are discussed below. The information associated with data sources was not released here because the discussion of MOM scenarios may imply that some existing practices might have negative effects on the environment, which might never exist. To evaluate how much difference that MOM made from the original management practices at the same ground, all compared data are simulation results based on the original management practices or MOM suggested management. Profit ($ ha^{-1}) in MOM is simply calculated by

$$
\begin{aligned}
Profit = {} & MarketValue \cdot CropYield / (1 + LoanInterest) \\
& - Price_{Fertilizer} \cdot Amount_{Fertilizer} \\
& - Price_{Water} \cdot Amount_{Irrigation} \cdot 10\ t\ ha^{-1}/mm \\
& - Cost_{FertilizerToFarm} \\
& - Cost_{(FertilizerToField + LaborToApply)} \cdot Applications_{Fertilizer} \\
& - Cost_{(WaterToField + LaborToIrrigate)} \cdot Applications_{Irrigation} \\
& - Cost_{FertilizerInIrrigation} \cdot Applications_{FertilizerInIrrigation} \\
& - OtherCost
\end{aligned}
$$

The economic factors and units in scenarios were assumed as follows:

$$
\begin{aligned}
MarketValue &= 0.50\ \$\ kg^{-1} \\
LoanInterest &= 12\ \%\ year^{-1} \\
Price_{Fertilizer} &= 0.80\ \$\ kgN^{-1} \\
Price_{Water} &= 0.05\ \$\ tonne^{-1} \\
Cost_{FertilizerToFarm} &= 5.00\ \$\ ha^{-1}
\end{aligned}
$$

$Cost_{(FertilizerToField\ +\ LaborToApply)}$ $= 5.00 + 100.00\ \$\ ha^{-1}$

$Cost_{(WaterToField\ +\ LaborToIrrigate)}$ $= 0.00 + 0.20\ \$\ ha^{-1}$

$Cost_{FertilizerInIrrigation}$ $= 0.00\ \$\ ha^{-1}$

$OtherCost$ $= 350.00\ \$\ ha^{-1}$ (includes planting and harvest costs)

Note that the profit and economic factors here are simply set to estimate relative costs associated with management activities. They may not be complete nor involve all current marketing factors. MOM may consider these factors in further development with the assistance of agricultural economists. During the MOM optimization search, the three MOM sub-goals, high profits, high yields and less nitrate leaching, were assigned the same weights.

Scenario-1

This is an example of the cropping in a tropical wet season (udic soil moisture regime). MOM first examined the "native" water supply potential during the cropping season and determined the amounts and timing of supplemental irrigation to meet possible shortage of the crop requirements (Fig. 6-4.1.1). Recalling section 5-3.2.3, for the soil N or soil water supply potential, when the supply index is equal to 0, the soil supply is equal to the crop requirement. A line at the index of zero, called *sufficient line*, was drawn in diagrams of soil N or soil water supply analysis to indicate where the soil supply satisfies the crop requirement. The soil water supply indexes of three soil layers under "native" conditions were close to *sufficient line*, only slightly lower

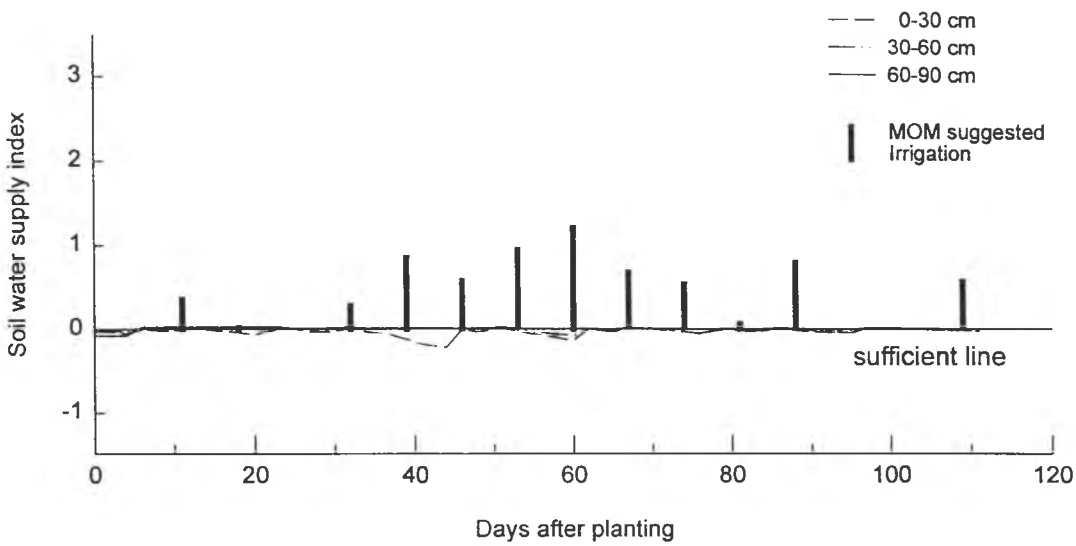


Fig. 6-4.1.1. Scenario-1. Soil water supply index analysis (See section 5-3.2.3) of the simulated "native" situation and MOM suggested irrigation schedule, during a wet cropping season.

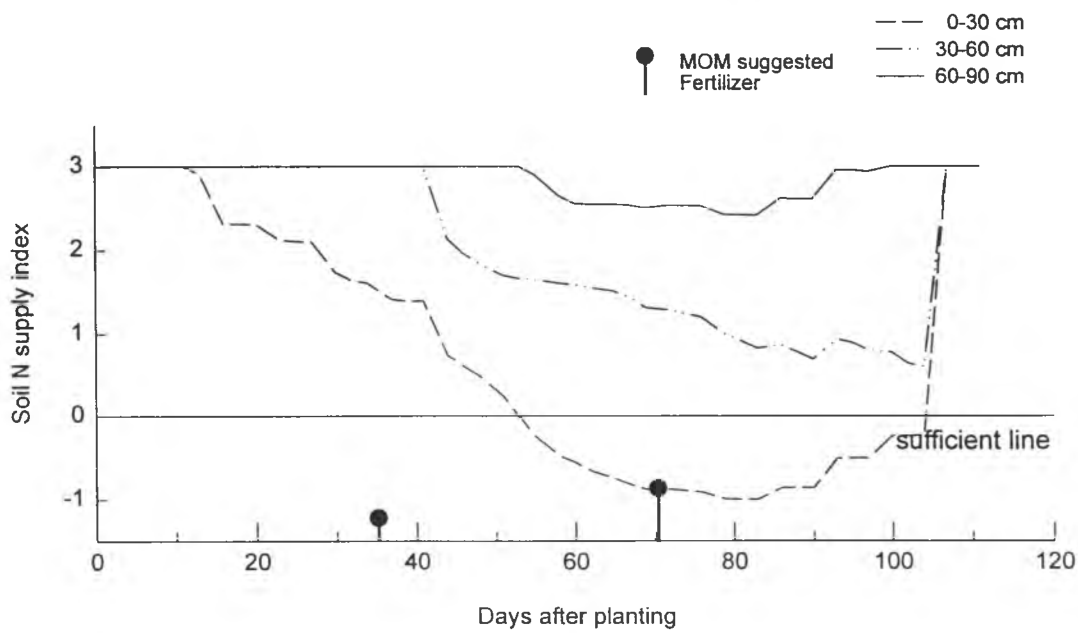


Fig. 6-4.1.2. Scenario-1. Soil N supply index analysis (See section 5-3.2.3) of the simulated "native" situation and MOM suggested N fertilization schedule, during a wet cropping season.

than it (Fig. 6-4.1.1). In other words, rainfall would provide most of the water the crop needs, so not much irrigation was needed. The "native" soil N supply potential was evaluated in Fig. 6-4.1.2. MOM predicted that N supply shortage in the major root zone would occur during the crop's rapid growth stage (about 50 - 100 days after planting), in which "native" soil N supply index of the surface layer (0-30 cm) was less than the *sufficient line*. So a small amount of N fertilizer was suggested shortly before and during this stage (Fig. 6-4.1.2). Measured soil nitrate contents at the beginning of cropping were 28 mg N kg^{-1} (about 92 kg N ha^{-1}, assuming soil BD = 1.1) in the major root zone (0-30 cm), 26 mg N kg^{-1} (about 85 kg N ha^{-1}) in the minor root zone (30-60 cm, assuming soil BD = 1.1), and 34 mg N kg^{-1} (about 123 kg N ha^{-1}, assuming soil BD = 1.2) in the transition zone (60-90 cm) in the scenario. Given the same goal weights to the three sub-goals of high profits, high yields and less nitrate leaching, MOM suggested 106 mm irrigation and 42 kgN ha^{-1} for the scenario (Table 6-4.1, Fig. 6-4.1.1 and Fig. 6-4.1.2). Based on the MOM suggested management, soil N supply potential during the cropping was simulated in Fig. 6-4.1.3. Comparing Fig. 6-4.1.3 with Fig. 6-4.1.2, the soil N supply index of the major root zone (0-30 cm) rose slightly over *sufficient line* after MOM suggested N fertilizer had been applied. It implies that MOM suggested management nearly matched the crop requirements during the growth. Inorganic N in the soil profile was simulated in Fig. 6-4.1.4. Inorganic N (mostly in nitrate form) concentration in the root zone became low at the end of the cropping. However, inorganic N remained high in the transition zone, where only a small fraction of the N was utilized by the crop. Inorganic N in the transition zone was a potential

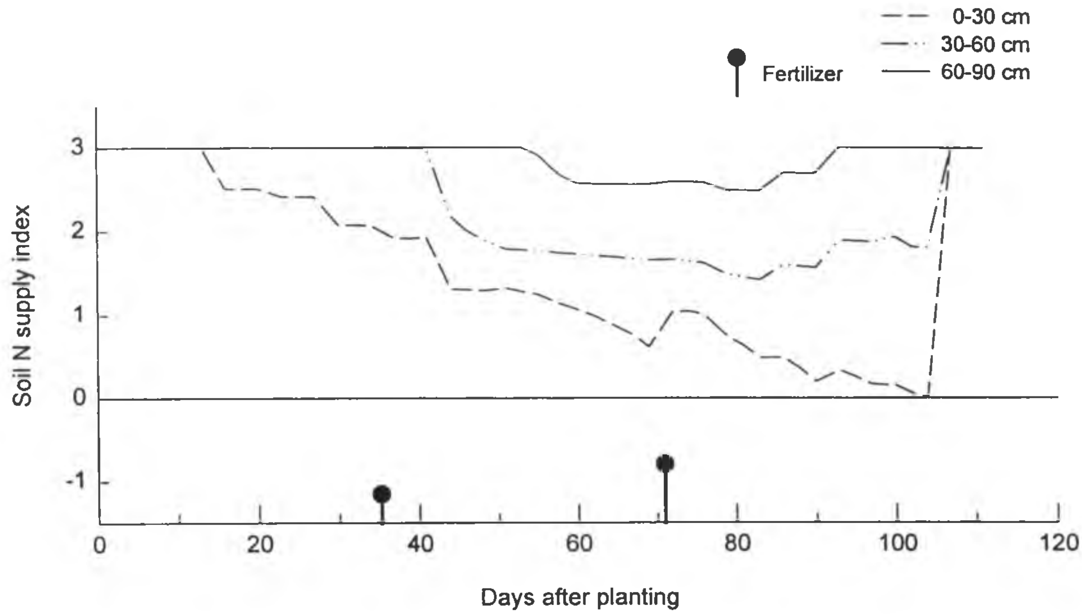


Fig. 6-4.1.3. Scenario-1. Soil N supply index analysis of the simulated situation under MOM-guided management schedule, during a wet cropping season.

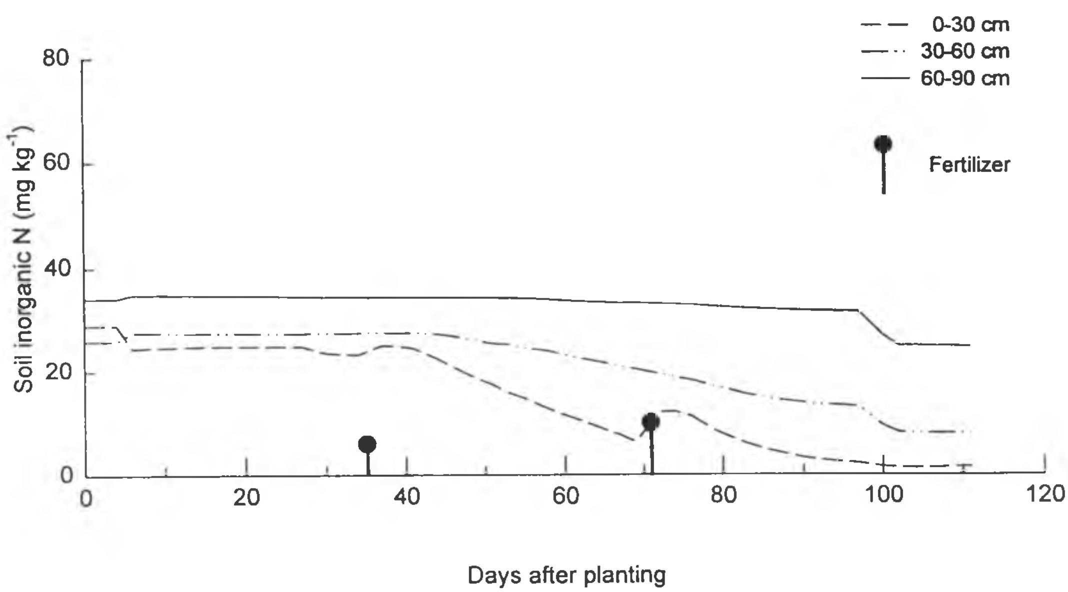


Fig. 6-4.1.4. Scenario-1. Simulated inorganic N (NO_3-N and NH_4-N) in the soil profile under MOM-guided management schedule, during a wet cropping season.

Table 6-4.1. MOM suggested N fertilization and irrigation schedule in scenario-1.

Week	Fertilizer *kgN ha⁻¹*	Irrigation *mm*
1	0.0	0.0
2	0.0	5.4
3	0.0	0.3
4	0.0	0.0
5	0.0	4.2
6	10.0	12.8
7	0.0	8.7
8	0.0	14.7
9	0.0	18.0
10	0.0	10.8
11	32.0	8.7
12	0.0	1.0
13	0.0	12.5
14	0.0	0.0
15	0.0	0.0
16	0.0	9.2
Sum	42.0	106.3

leaching source unless the following crops could develop deep roots in this layer. The large rain near the end of the cropping season might leach this inorganic N out of the root zone as occurred in scenario-1 (Fig. 6-4.1.5). Comparing simulation results (crop uptake N, percolation, and leachate nitrate) of the original management practice (Fig. 6-4.1.5) with those the MOM-suggested management (Fig. 6-4.1.6), it suggests that MOM recommendations had controlled much of the excessive percolation, which in turn reduced nitrate leaching. Although MOM could not control the severe leaching peak at 100 days after planting, which was caused by a large rain event, MOM had reduced the total of nitrate leaching from 175 kg N ha^{-1} to 67 kg N ha^{-1}. Compared to the original management, MOM also reduced costs by reducing the amounts and

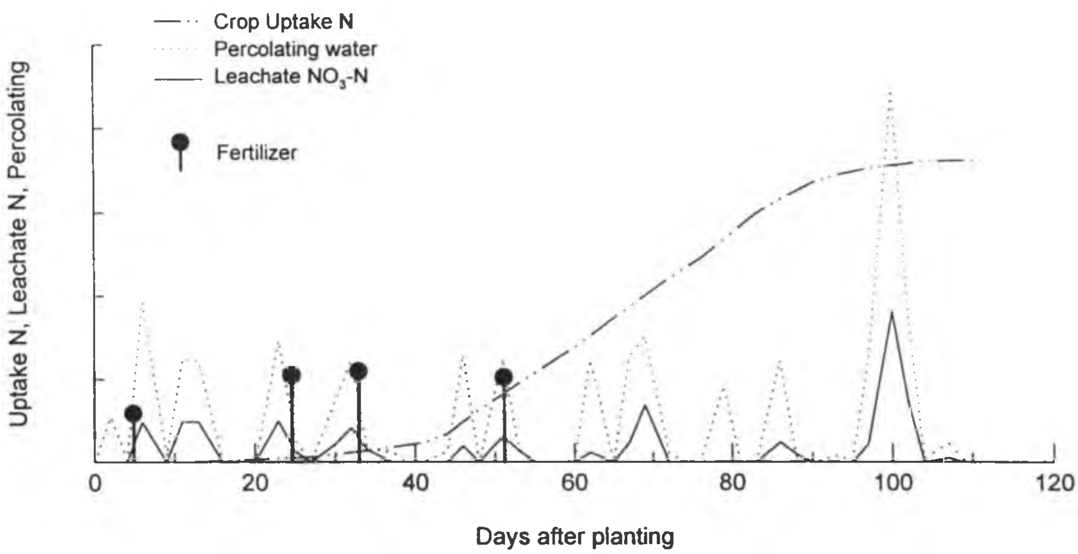


Fig. 6-4.1.5. Scenario-1. Simulated crop uptake N, leachate N, and percolating water under the original management conditions of the dataset, during a wet cropping season.

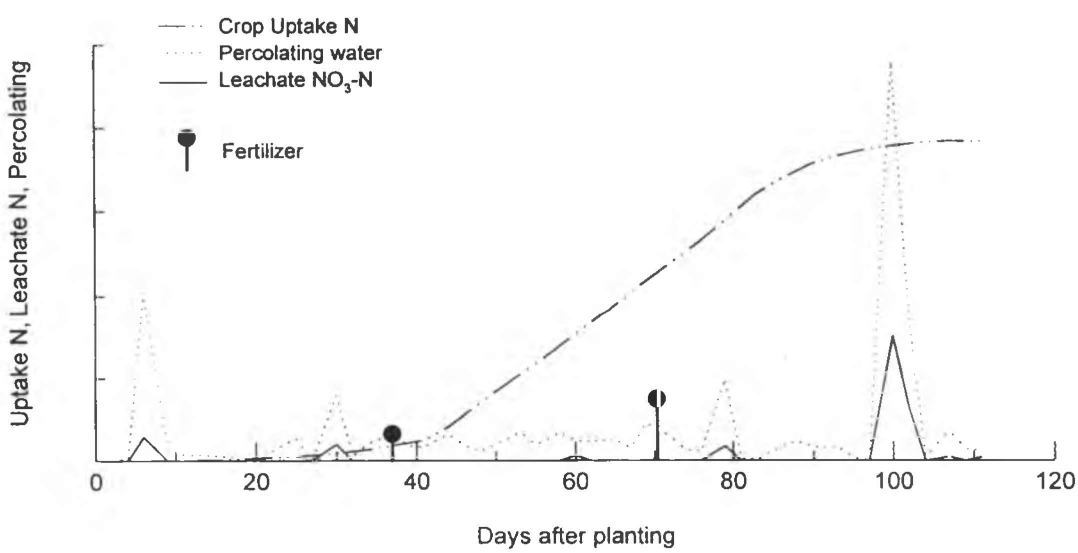


Fig. 6-4.1.6. Scenario-1. Simulated crop uptake N, leachate N, and percolating water under MOM-guided management schedule, during a wet cropping season.

applications of the fertilizer, while maintaining the yield. Finally, the MOM suggested management returned \$600 ha^{-1} more profit and 108 kg N ha^{-1} less nitrate leaching than the original management in scenario-1 (Table 6-4.2).

Table 6-4.2. Summary of five scenarios of MOM optimizing N management†

Scenario	Management	Profit *\$ ha⁻¹*	Yield *kg ha⁻¹*	Leachate N *kgN ha⁻¹*	Fertilizer *kgN ha⁻¹*	Irrigation *mm*
(1)	Original	3314	9092	175	200	323
	MOM	3986	9589	67	42	106
(2)	Original	3697	9728	40	197	387
	MOM	4439	11001	8	224	271
(3)	Original	1063	4212	5	200	239
	MOM	3414	9007	2	150	298
(4)	Original	1785	4709	96	10	0
	MOM	3852	10101	103	224	234
(5)	Original	2711	6645	102	10‡	0
	MOM	4152	10318	115	111‡	234

† All data of profit, yield, and leachate N are results simulated by N-SIMULATOR. Fertilizer and Irrigation data come from original datasets or MOM suggestions.

‡ Approximate 180 kgN ha^{-1} of legume manure was applied preplant. The cost of the manure was not included in the analysis.

Scenario-2

Scenario-2 represents cropping during a tropical dry season. The "native" water supply potential of the scenario was simulated in Fig. 6-4.2.1, with a primary irrigation schedule that MOM suggested to match the crop requirements. Fig. 6-4.2.1 shows that the water supply in the major root zone was insufficient and MOM recommended more irrigation for the crop during this dry season than that in scenario-1 (wet season). Fig. 6-4.2.2 illustrates the "native" soil N supply potential of the site during cropping and MOM suggested N fertilization during the crop rapid growth period. The soil nitrate

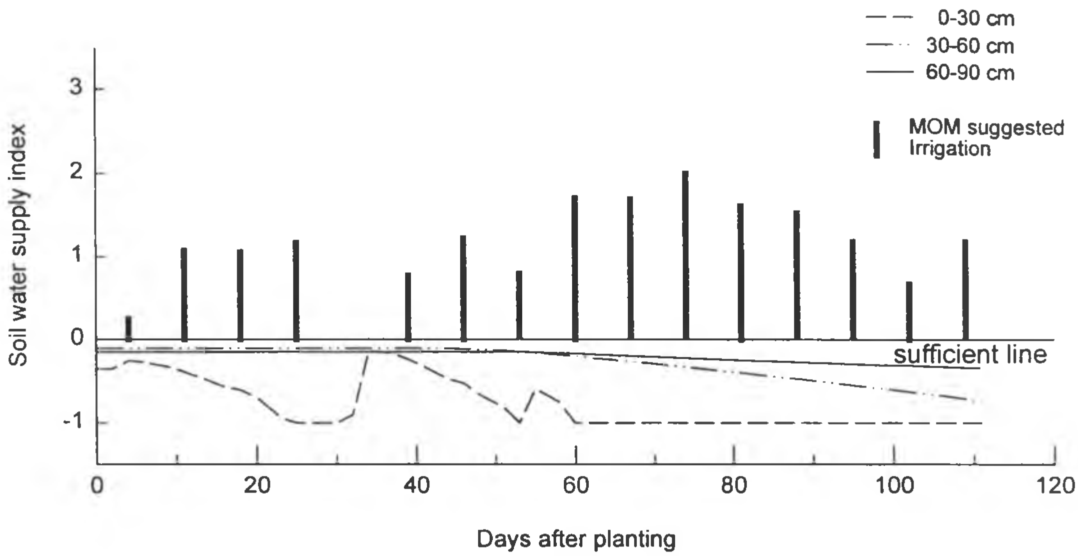


Fig. 6-4.2.1. Scenario-2. Soil water supply index analysis of the simulated "native" situation and MOM-guided irrigation schedule, during a dry cropping season.

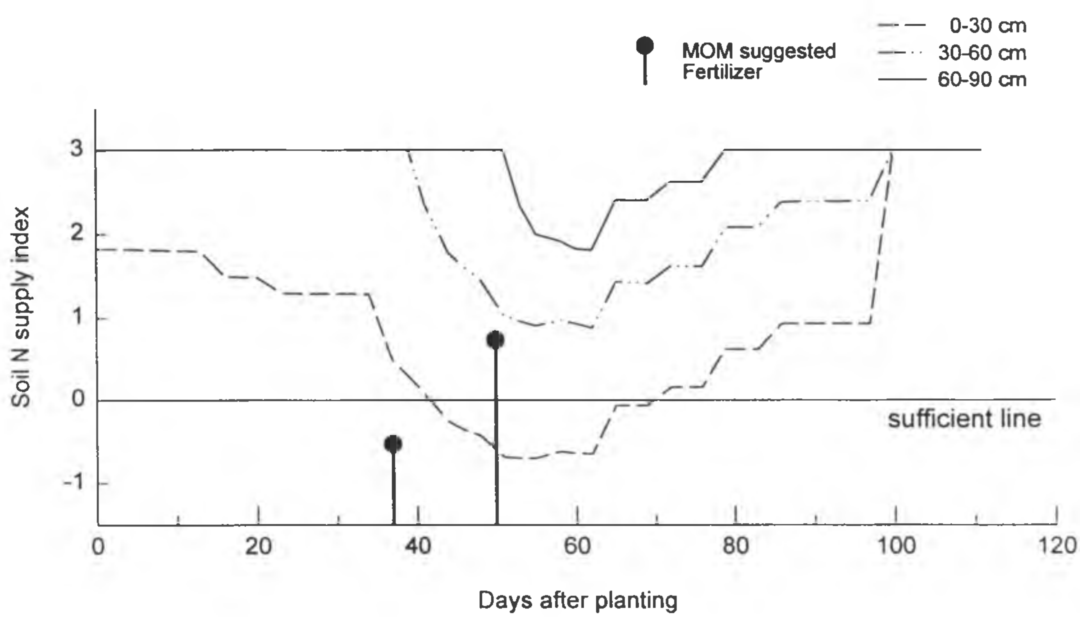


Fig. 6-4.2.2. Scenario-2. Soil N supply index analysis of the simulated "native" situation and MOM-guided N fertilization schedule, during a dry cropping season.

contents at the beginning of cropping were 10 mg N kg^{-1} (about 34 kg N ha^{-1}, assuming soil BD = 1.1) in the major root zone (0-30 cm), 11 mg N kg^{-1} (about 37 kg N ha^{-1}) in the minor root zone (30-60 cm, assuming soil BD = 1.1), and 15 mg N kg^{-1} (about 52 kg N ha^{-1}, assuming soil BD = 1.2) in the transition zone (60-90 cm). Initial soil inorganic N of the scenario was less than that of scenario-1. More fertilizer and irrigation, 224 kg N ha^{-1} with 271 mm irrigation in total, were suggested for the scenario-2 (timing shown in Fig. 6-4.2.1 and Fig. 6-4.2.2). Soil N supply potential under MOM management was simulated in Fig. 6-4.2.3 and soil inorganic N was simulated in Fig. 6-4.2.4. Inorganic N in the soil profile increased during crop growth but after harvest returned to approximate the same levels as before planting. No extra inorganic N was accumulated in the root zone under MOM suggested management. Fig. 6-4.2.5 shows crop uptake N, percolation, and leachate nitrate of original management practice and Fig. 6-4.2.6 shows the same measurements under MOM suggested management. Simulated profit, yield and leachate nitrate of the scenario were listed in Table 6-4.2. Except for some savings in irrigation, the original management practice was close to MOM suggestion. MOM would not have greatly improved profit and yield in this scenario. However, some reduction in nitrate leaching, from 40 kg N ha^{-1} to 8 kg N ha^{-1}, was predicted. Scenario-1 and scenario-2 demonstrate that careful N management is necessary to minimize nitrate leaching for cropping in a tropical wet season. With uncertain rainfall, that is a difficult management objective even with a decision-aid.

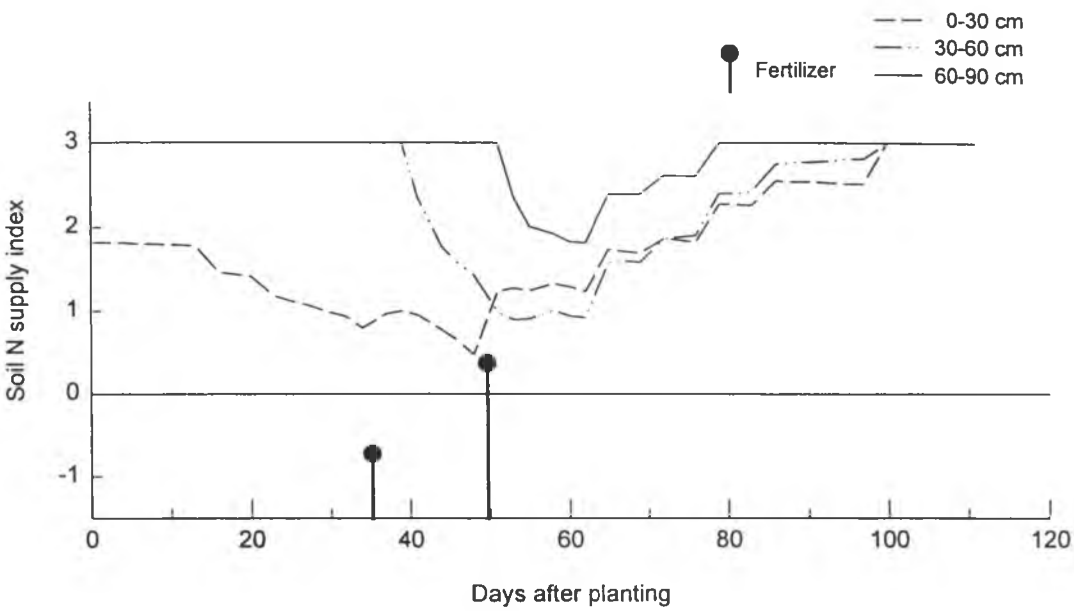


Fig. 6-4.2.3. Scenario-2. Soil N supply index analysis of the simulated situation under MOM-guided management schedule, during a dry cropping season.

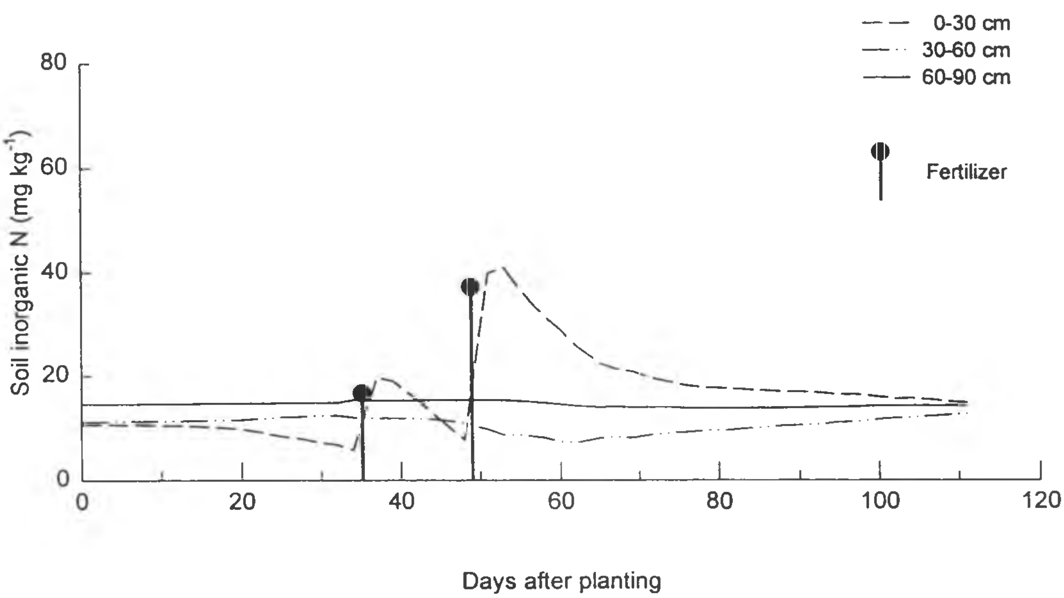


Fig. 6-4.2.4. Scenario-2. Simulated inorganic N (NO_3-N and NH_4-N) in the soil profile under MOM-guided management schedule, during a dry cropping season.

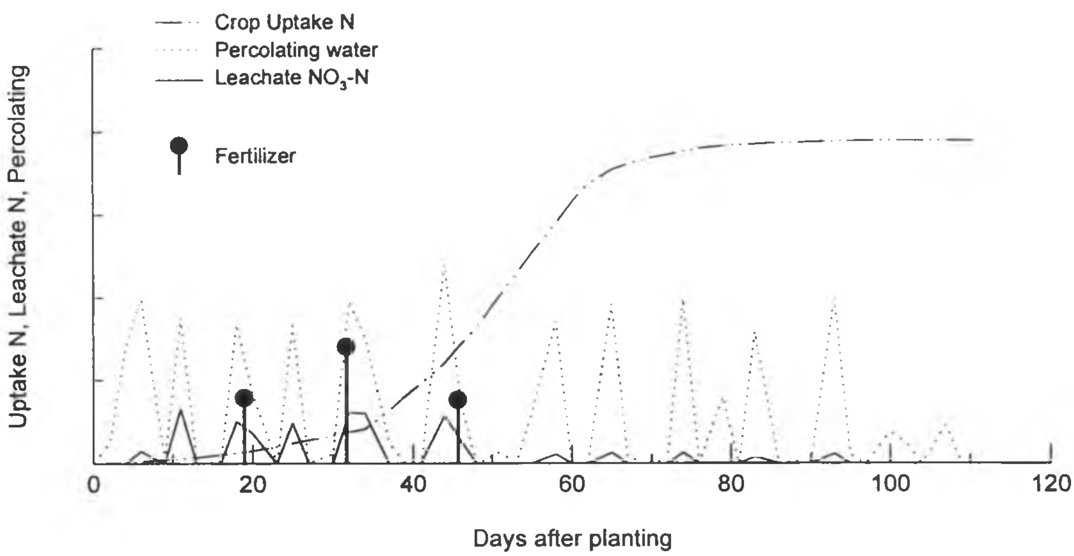


Fig. 6-4.2.5. Scenario-2. Simulated crop uptake N, leachate N, and percolating water under the original management conditions of the dataset, during a dry cropping season.

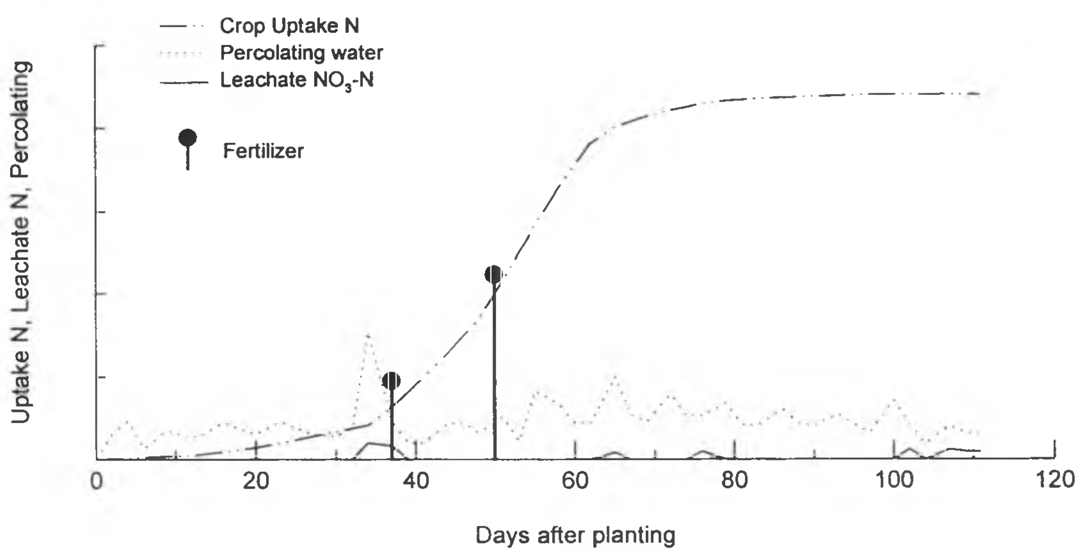


Fig. 6-4.2.6. Scenario-2. Simulated crop uptake N, leachate N, and percolating water under MOM-guided management schedule, during a dry cropping season.

Scenario-3

In contrast with first two scenarios, initial concentration of inorganic N in the soil profile in scenario-3 was very low (Fig. 6-4.3.4). The "native" water supply potential analysis (Fig. 6-4.3.1) shows that the crop needs to be well irrigated in the scenario. This is also an only scenario in which "native" soil N supply potential of the subsoil layers (30-90 cm) fell below the crop requirements during the rapid growth period (Fig. 6-4.3.2). Fig. 6-4.3.3 shows soil N supply potential during the cropping. The concentration of inorganic N in the soil profile rose during the crop growth and finally returned to the low levels that were close to initial levels (Fig. 6-4.3.4). Fig. 6-4.3.5 shows crop uptake N, percolation, and leachate nitrate of the original management practice and Fig. 6-4.3.6 shows those of MOM suggested management. MOM suggested less N fertilizer but more irrigation than the original management. Simulated results show that MOM obtained higher profit and yield than the original management (Table 6-4.2). This may be explained by Fig. 6-4.3.5 and Fig. 6-4.3.6, which illustrate that MOM provided a more stable water supply than the original management. It implies that water was a major restrictive factor in scenario-3. Low rates of leachate nitrate in both management practices in the scenario might be due to low nitrate in the transition zone.

Scenario-4 and Scenario-5

Original cropping practices in scenario-4 and scenario-5 were rainfed with 10 kg N ha^{-1} inorganic fertilizer preplant. Approximately 180 kg N ha^{-1} of legume manure was applied preplant in scenario-5. Scenario-4 was nearly a "native" case and scenario-

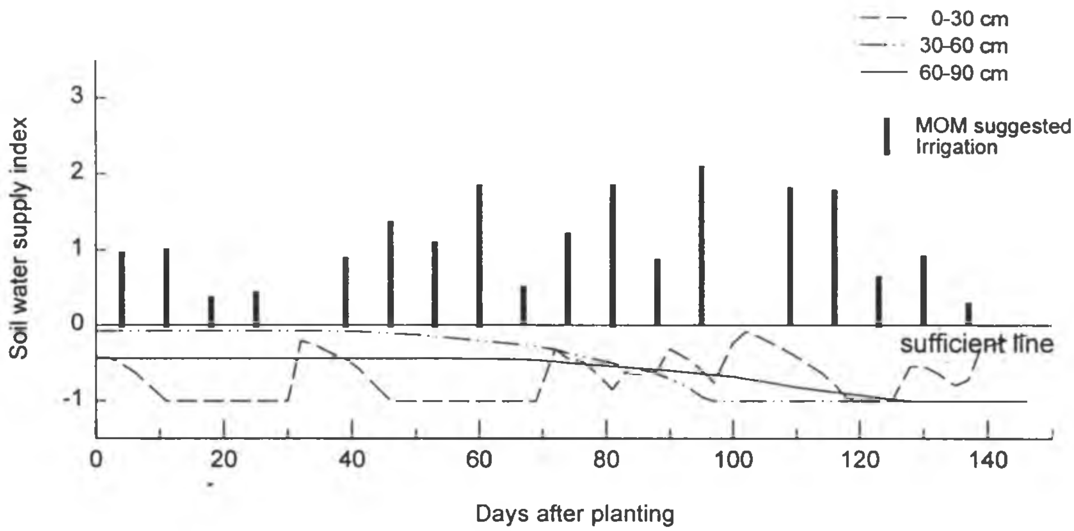


Fig. 6-4.3.1. Scenario-3. Soil water supply index analysis of the simulated "native" situation and MOM-guided irrigation schedule, during the cropping season.

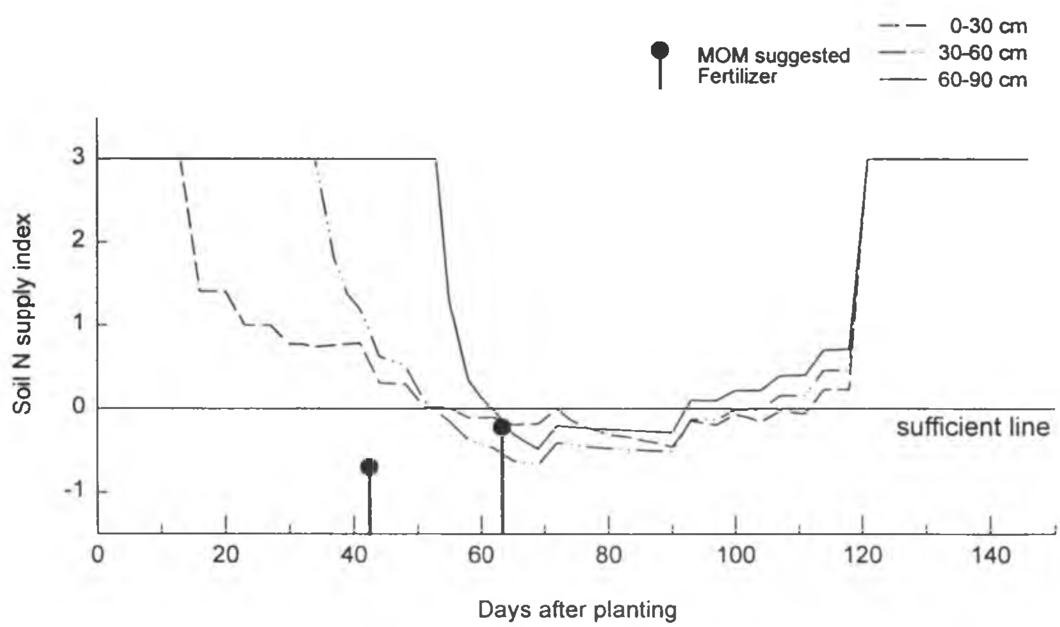


Fig. 6-4.3.2. Scenario-3. Soil N supply index analysis of the simulated "native" situation and MOM-guided N fertilization schedule, during the cropping season.

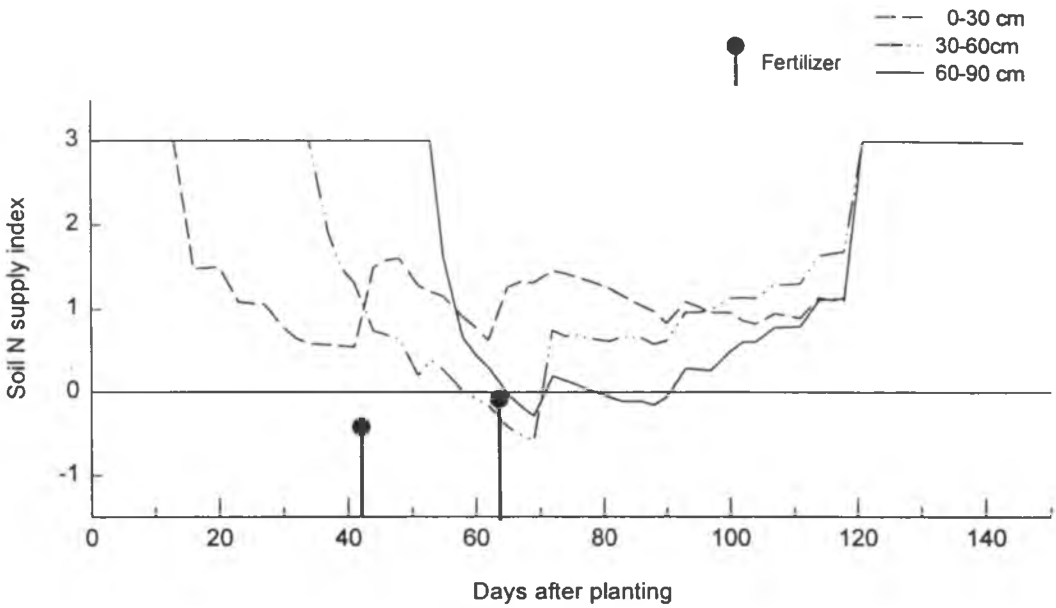


Fig. 6-4.3.3. Scenario-3. Soil N supply index analysis of the simulated situation under MOM-guided management schedule, during the cropping season.

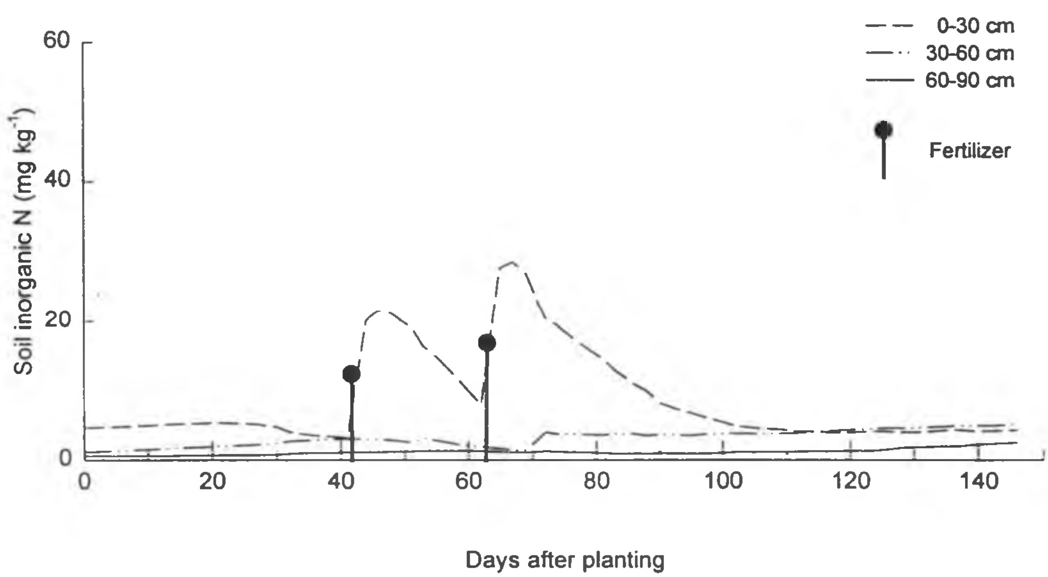


Fig. 6-4.3.4. Scenario-3. Simulated inorganic N (NO_3-N and NH_4-N) in the soil profile under MOM suggested management schedule, during the cropping season.

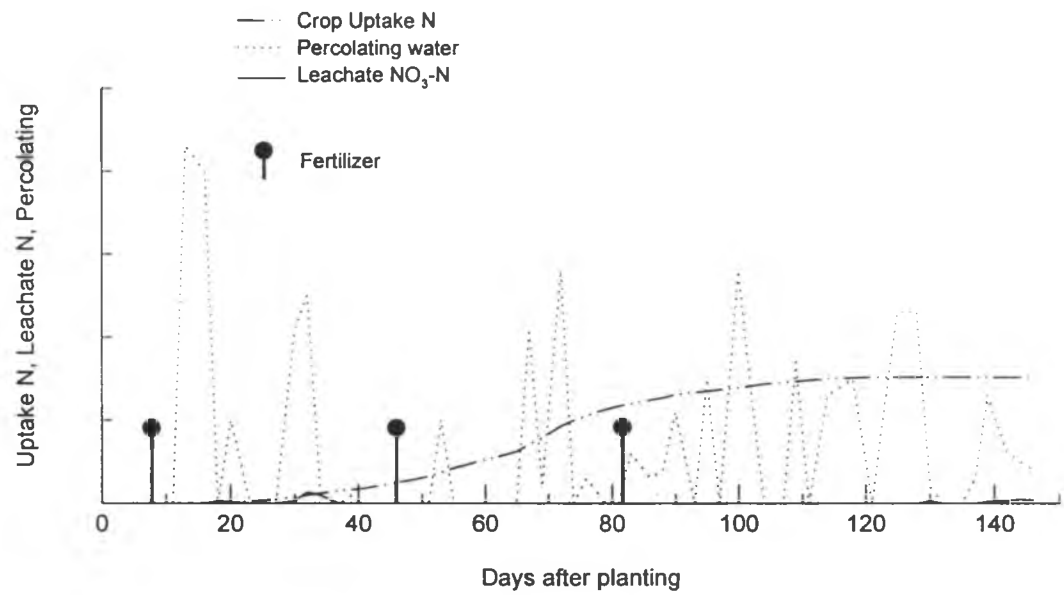


Fig. 6-4.3.5. Scenario-3. Simulated crop uptake N, leachate N, and percolating water under the original management conditions of the dataset, during the cropping season.

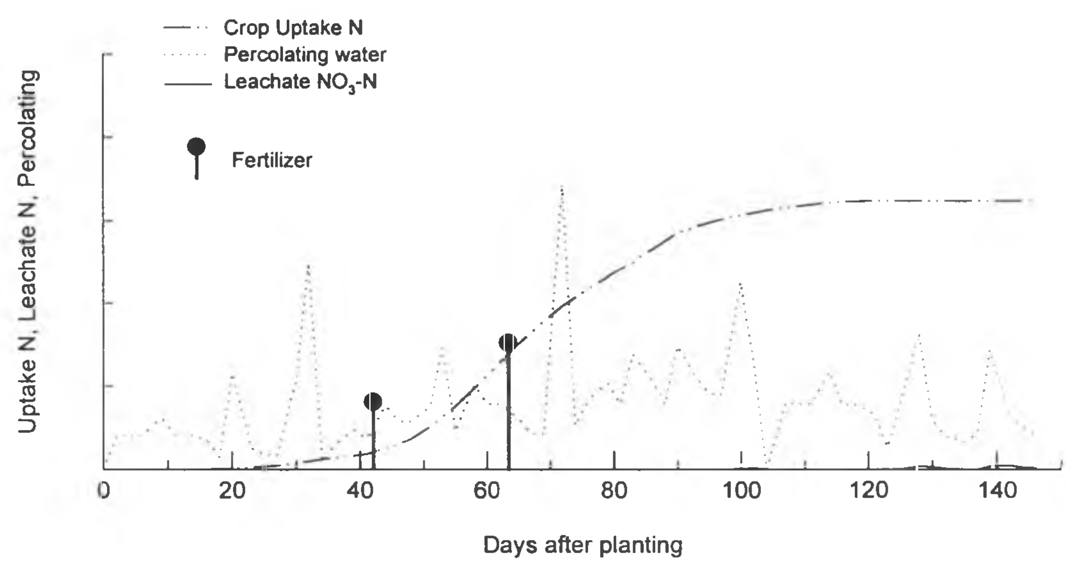


Fig. 6-4.3.6. Scenario-3. Simulated crop uptake N, leachate N, and percolating water under MOM-guided management schedule, during the cropping season.

5 is an example of organic farming. They are good cases to evaluate MOM in optimizing management for profit by fertilization and irrigation, and to test MOM's capability of incorporating inorganic and organic farming practices. For scenario-4, "native" water supply potential, soil N supply potential, and soil inorganic N were simulated in Fig. 6-4.4.1, Fig. 6-4.4.2, Fig. 6-4.4.3, and Fig. 6-4.4.4. Crop N uptake, percolation, and leachate nitrate for both the original management practice and MOM suggested management are shown in Fig. 6-4.4.5 and Fig. 6-4.4.6. The same diagrams for scenario-5 are given in Fig. 6-4.5.1, Fig. 6-4.5.2, Fig. 6-4.5.3, Fig. 6-4.5.4, and Fig. 6-4.5.5. Simulated profits, yields and nitrate leaching rates of both scenarios are listed in Table 6-4.2. Comparing scenario-4 with scenario-5, one can conclude that (1) Both inorganic farming and inorganic combined with organic farming would profit from the management MOM suggested. The simulation suggests that the crop yield under combined farming was slightly higher than that under inorganic farming. (2) MOM would detect when and how much inorganic N can be released from preplant legume manure and match appropriate inorganic fertilizer for crop growth requirements. (3) Both scenarios show high rates of nitrate leaching at almost "native" conditions, but MOM could not help much in reducing them. Initial soil nitrate contents in the major root zone (0-30 cm), the minor root zone (30-60 cm), and the transition zone (60-90 cm) were 5.0, 4.5, 27 mg N kg^{-1} for scenario-4, and 9.4, 4.5, 30 mg N kg^{-1} for scenario-5. The distributions show approximate 75% of the initial soil nitrate was stored so deep that most crop roots could not reach it. Assuming that soil BD = 1.2 in the transition zone (60-90 cm), the amount of nitrate accumulated in the layer contained

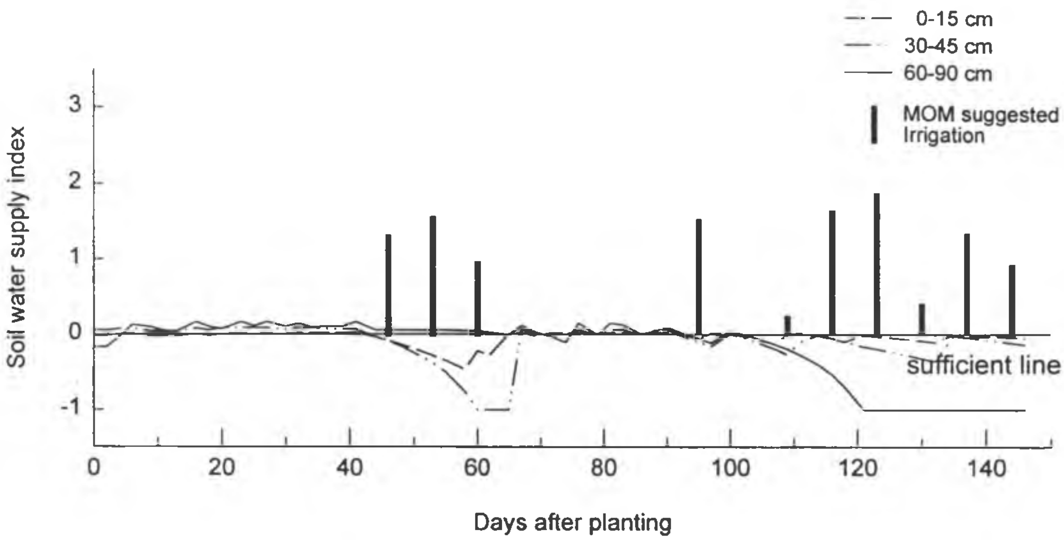


Fig. 6-4.4.1. Scenario-4. Soil water supply index analysis of the simulated "native" situation and MOM-guided irrigation schedule, during a wet cropping season.

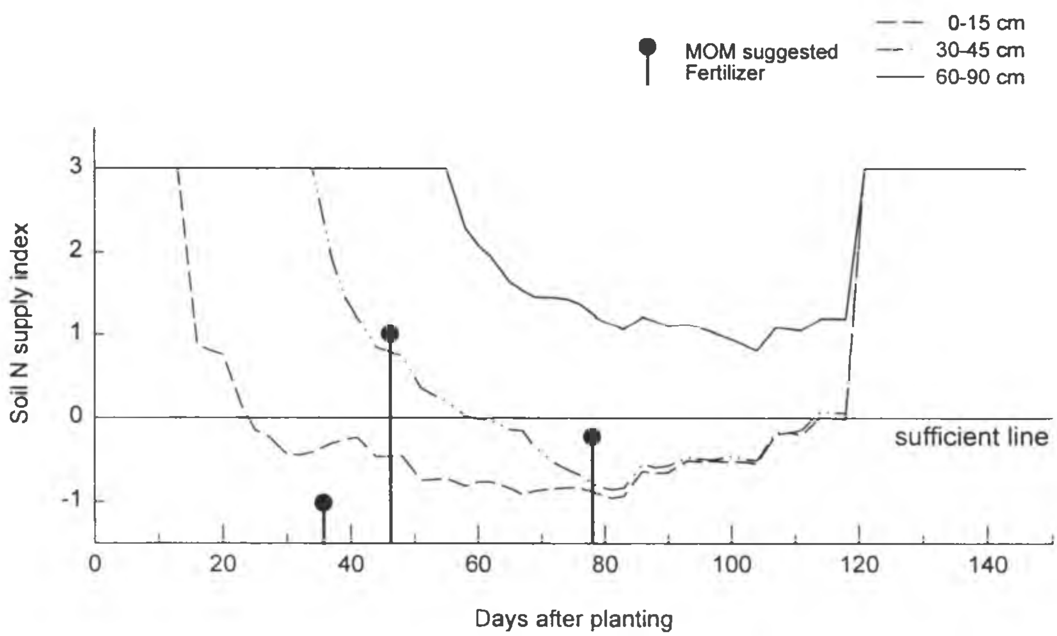


Fig. 6-4.4.2. Scenario-4. Soil N supply index analysis of the simulated "native" situation and MOM-guided N fertilization schedule, during a wet cropping season.

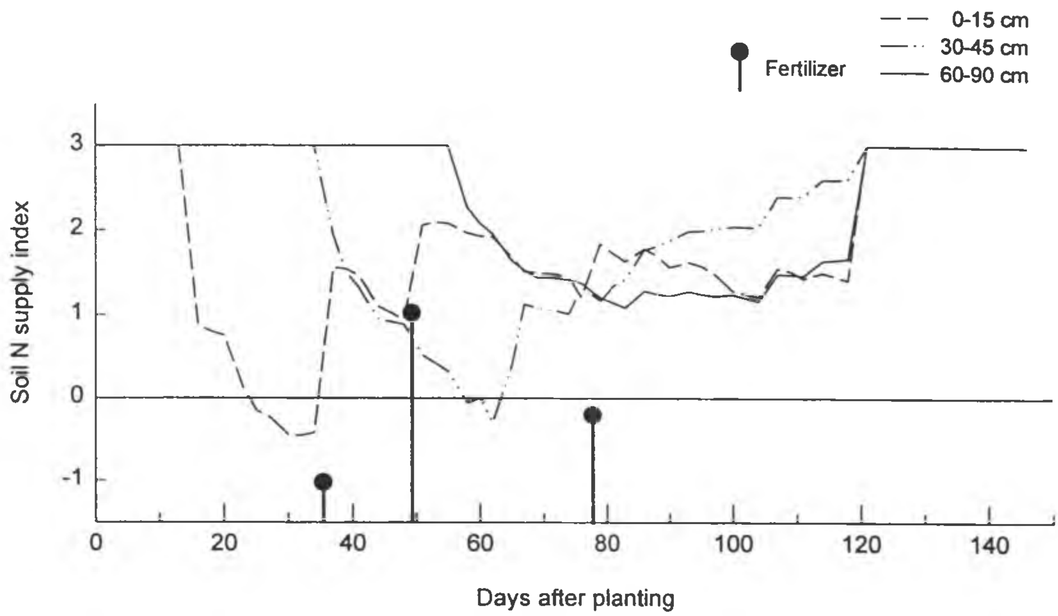


Fig. 6-4.4.3. Scenario-4. Soil N supply index analysis of the simulated situation under MOM-guided management schedule, during a wet cropping season.

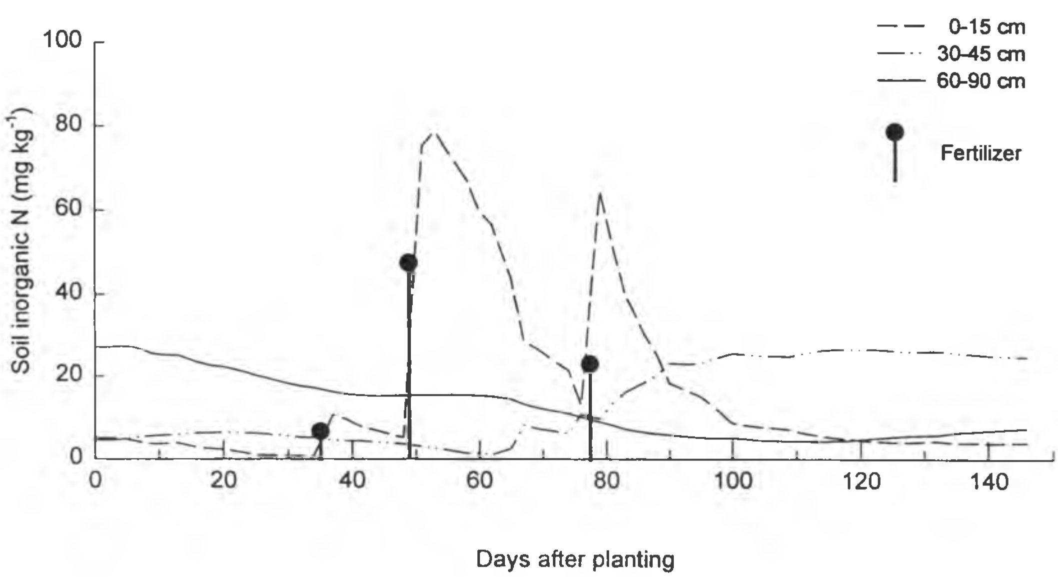


Fig. 6-4.4.4. Scenario-4. Simulated inorganic N (NO_3-N and NH_4-N) in the soil profile under MOM suggested management schedule, during a wet cropping season.

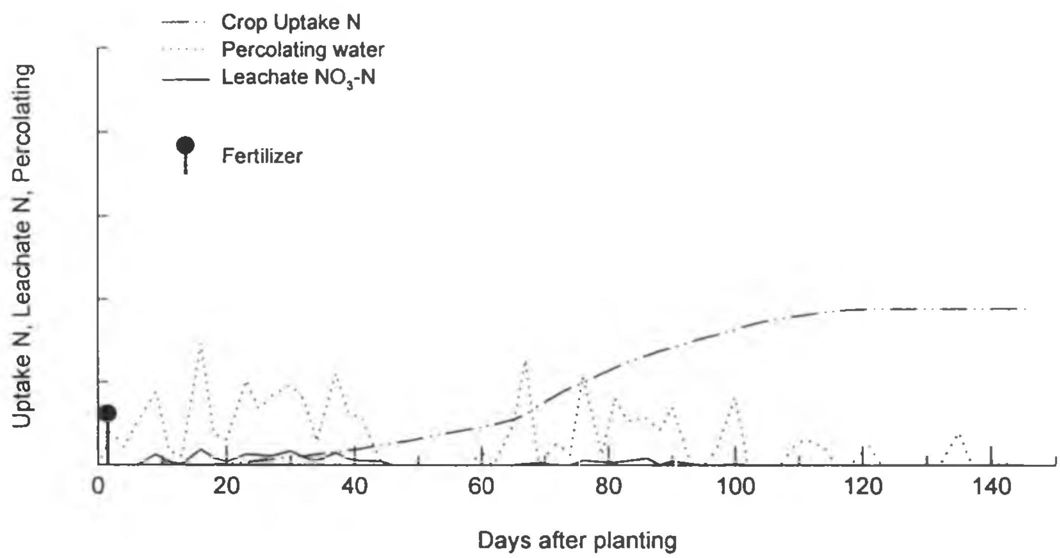


Fig. 6-4.4.5. Scenario-4. Simulated crop uptake N, leachate N, and percolating water under the original management conditions of the dataset, during a wet cropping season.

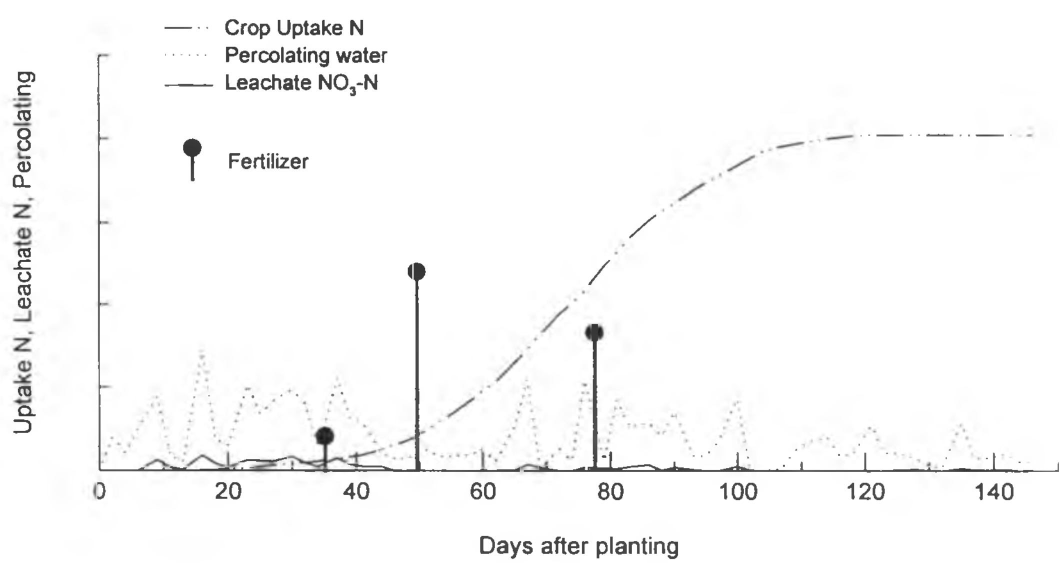


Fig. 6-4.4.6. Scenario-4. Simulated crop uptake N, leachate N, and percolating water under MOM-guided management schedule, during a wet cropping season.

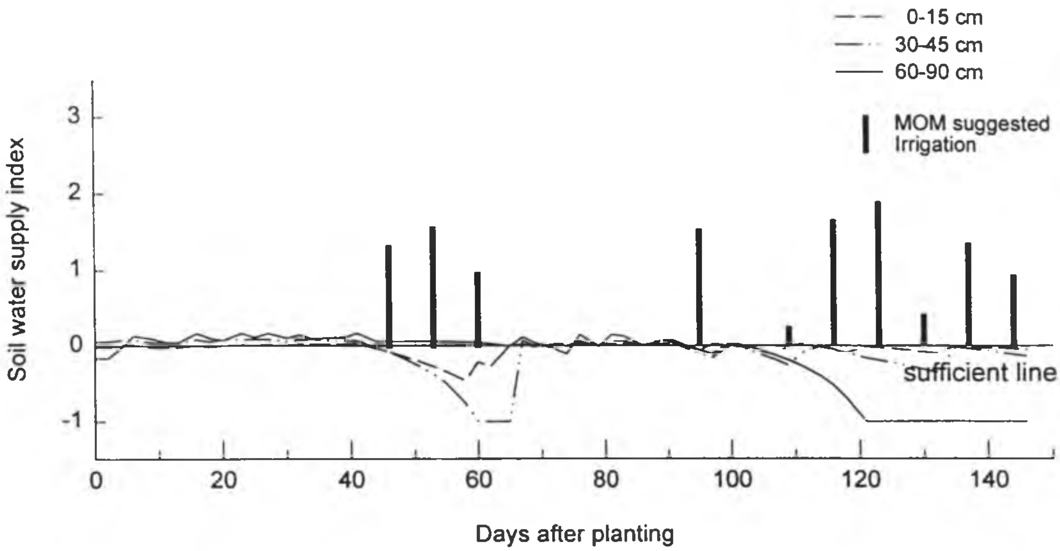


Fig. 6-4.5.1. Scenario-5. Soil water supply index analysis of the simulated "native" situation and MOM-guided irrigation schedule (legume manure applied preplant), during a wet cropping season.

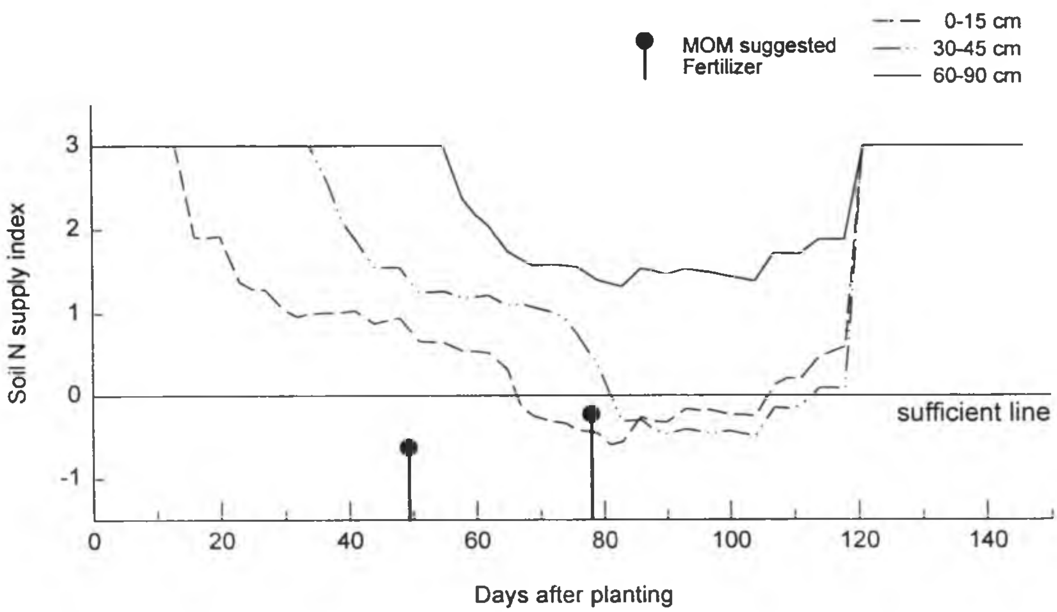


Fig. 6-4.5.2. Scenario-5. Soil N supply index analysis of the simulated "native" situation and MOM-guided N fertilization schedule (legume manure applied preplant), during a wet cropping season.

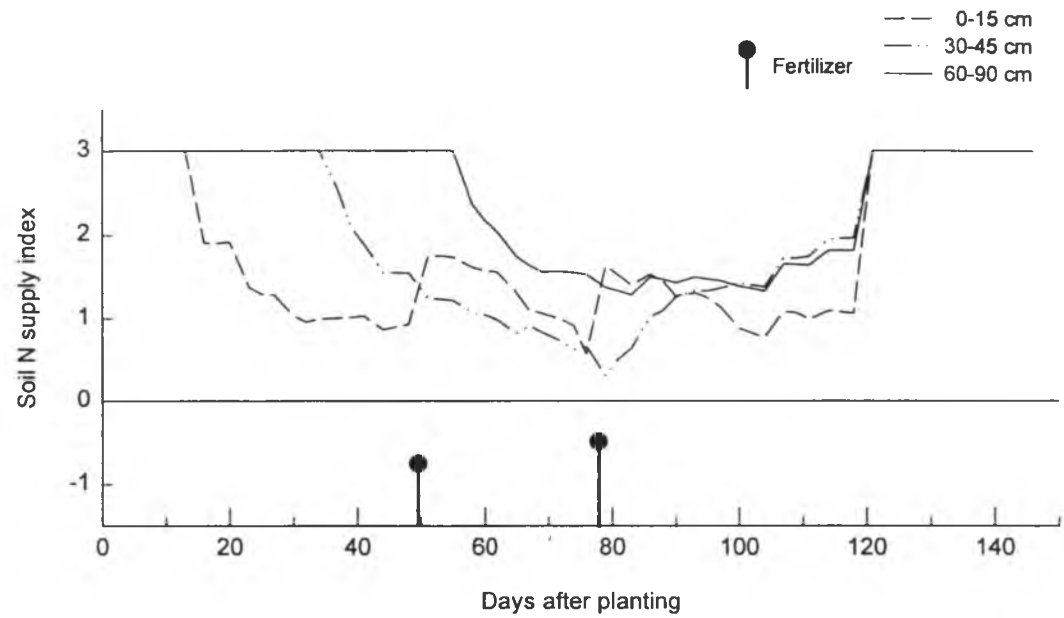


Fig. 6-4.5.3. Scenario-5. Soil N supply index analysis of the simulated situation under MOM-guided management schedule (legume manure applied preplant), during a wet cropping season.

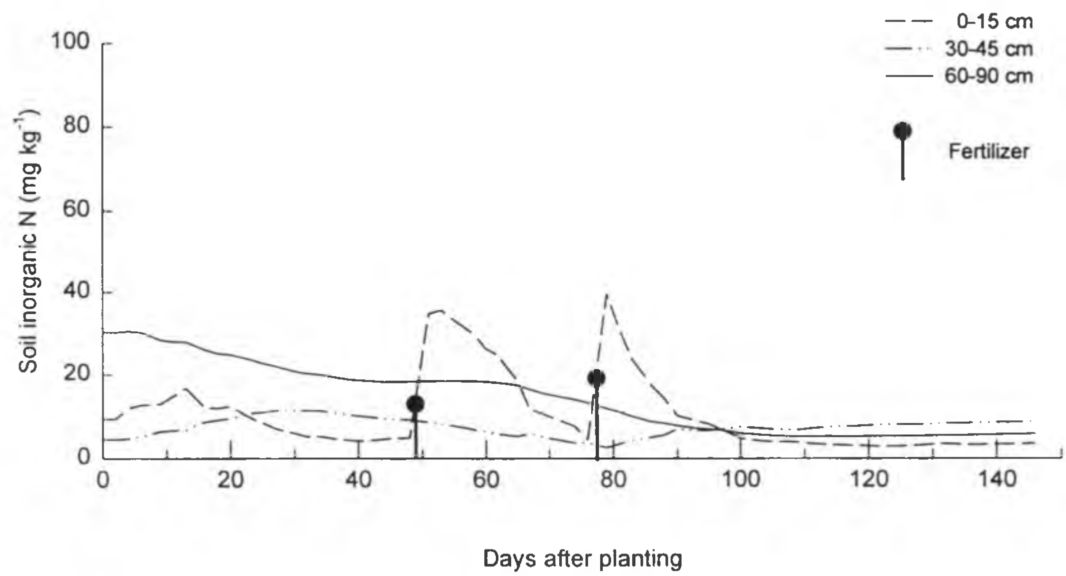


Fig. 6-4.5.4. Scenario-5. Simulated inorganic N (NO_3-N and NH_4-N) in the soil profile under MOM suggested management schedule (legume manure applied preplant), during a wet cropping season.

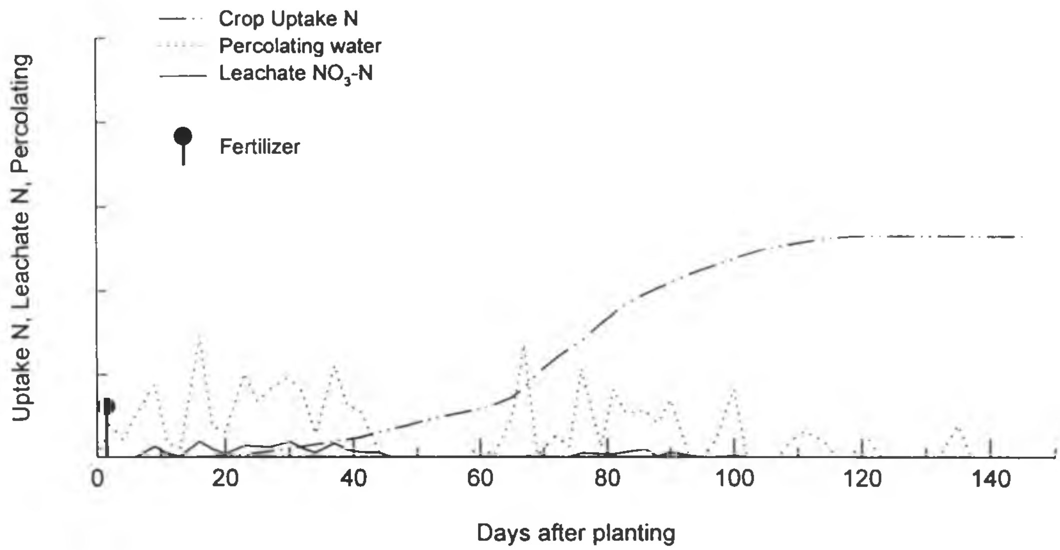


Fig. 6-4.5.5. Scenario-5. Simulated crop uptake N, leachate N, and percolating water under the original management conditions of the dataset (legume manure applied preplant), during a wet cropping season.

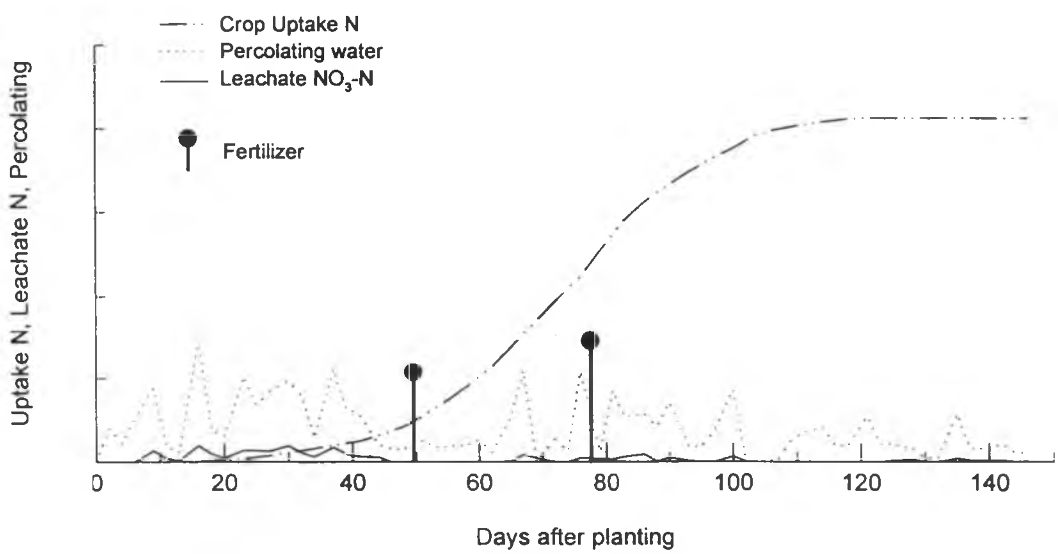


Fig. 6-4.5.6. Scenario-5. Simulated crop uptake N, leachate N, and percolating water under MOM-guided management schedule (legume manure applied preplant), during a wet cropping season.

approximately 97 kg N ha^{-1} for scenario-4 and 108 kg N ha^{-1} for scenario-5. These numbers are very close to the numbers of simulated "native" nitrate leaching in Table 6-4.2. It implies that this kind of "native" leaching may be due to accumulated nitrate in deep soil layers drained by tropical rainfall in the wet season. The accumulated nitrate in deep soil layers may have resulted from previous mismanagement of fertilizer.

6-5. Summary

Within-season management decision aids are important for precision nitrogen management because the final fate of the N in soil-plant systems largely depends on within-season events and management. Uncertainty in future weather challenges N models for within-season management. While weather generators can simulate weather they do not predict weather for a given season. Nitrogen sensors monitor crop N by color, not soil N content. Although N sensors have been useful for some crops to monitor N fertilization based on tissue N deficiency, their recommendation of fertilization occurs too late to optimize within-season management for many crops, because normal growth of the crops require sufficient N supply before the N deficiency occurs.

After correctly calibrated and validated to specific sites and crops, MOM should be a useful tool to guide within-season nitrogen management. MOM uses weather forecasts to estimate rainfall in the near future and simulates other components in the soil-plant systems. In addition to its management-oriented optimization, MOM-guided within-season management has the advantages of (1) High efficiency in predicting timely information. Users are advised of the probable status of soil-plant systems in advance of sensors and soil tests. (2) Low cost to implement. No within-season soil or tissue sampling and testing are required except an initial soil test. (3) "Transparency" of the systems' status. Daily descriptions of the N cycle in soil-plant systems during the cropping season graphically advise users how to control the fate of nitrogen. MOM also presents within-season estimates of leachate nitrate and mineralized N, which are not provided by standard soil tests. Within-season observed data of precipitation and crop growth update MOM-guided management with current events, which improve precision that MOM traces the N cycle in soil-plant systems.

MOM-guided within-season management was not designed to match future events exactly, but to dynamically adjust probable consequences of management strategies to fit changing conditions within a cropping season. Although MOM has been only partially validated, e.g., its simulator, the scenarios suggest that MOM can help in precision nitrogen management for maximizing profits and yields while minimizing nitrate leaching by updating management of irrigation and fertilization within-season.

Chapter 7

Summary

Precision nitrogen management has developed rapidly in recent years due to impact of nitrogen on the environment. Nitrogen models are important tools for precision management. Nine existing N models were evaluated in assessing the state-of-the-art of N modeling. These models were designed to *describe* the N status in soil-plant systems, but not to *change* the situation by modeling the management alternatives and choices. To model nitrogen management, Management-Oriented Modeling (MOM), a dynamic simulation modeling using artificial intelligence (AI) optimization techniques, has been developed in this study. MOM provides a precision tool in finding optimal solutions for N management to minimize nitrate leaching and maximize production and profits. The model was calibrated and validated with 11 datasets from Hawaii and Brazil. Results show that the model accuracy of simulating the N cycle in soil-plant systems was acceptable for field N management.

This study provided an alternate modeling framework in quantitatively optimizing nitrogen management activities with AI technologies. MOM consists of a generator, a simulator, and an evaluator. The generator produces a group of best guess nodes of management strategies. The simulator predicts the results of the nodes. The evaluator uses the built-in knowledge and interaction with the user to analyze the outputs of the simulator and to guide the generator in producing nodes. A mixed search method, *hill-climbing* as a strategic search method that embraces *best-first* as a tactical search method, was developed to find the shortest path from the start nodes to goals. MOM (Management-Oriented Modeling) is an example of goal-driven modeling in which the simulation is directed toward user-weighted goals. The model can be used as a tactical N management tool for within-season management of specific conditions and used as a strategic N management tool for general decision rules. As a tool guiding nitrogen within-season management, MOM simulates the activities of fertilization and irrigation and the consequences in soil-plant systems, based on weather forecasting of rainfall in the near future. In addition to management-oriented optimization, MOM within-season management provides users with daily "pictures" of the N status in soil-plant systems in-season without sampling and testing. Scenarios suggest that MOM can help in precision nitrogen management for maximizing profits and yields while minimizing nitrate leaching by updating management of irrigation and fertilization within-season. In addition, MOM has been developed as stand alone Windows software in this study.

Appendix A

Major Source Code[1]

1. Generator

```
procedure DetermineWeekIrrigation;
{-----------------------------------
Input       Soil, Plant, Rainfall data.  Assume N uptake = plant demanded.
Output      Weekly irrigation rates WaterNeeded[weeks]
}
var I : Integer;
begin
for I := 1 to TimeStep do DailyIrrgFraction[I] := 1.0/TimeStep; {assume irrigate every
day}
for I := 1 to TotalGrowWeek do WaterNeeded[I] := 0.0;
SoilWaterN_Simulation(DetectWater, 0, 0, 0);
end;

procedure DetermineWeekFertilizer;
{-----------------------------------
Input    Soil, Plant, Rainfall, WaterNeeded, let soil water close to 90% of DrainLmt.
Output   Weekly N fertilizer Needed: N_Needed[weeks]
}
var  I : Integer;
begin
for I := 1 to TimeStep do DailyIrrgFraction[I] := 1.0/TimeStep; {assume irrigate every
day}
for I := 1 to TotalGrowWeek do N_Needed[I] := 0.0;
SoilWaterN_Simulation(DetectN, 0, 0, 0);
end; {DetermineWeekFertilizer}

Procedure EstimateWaterNeededThisWeek(EP_panWk, LAI_Actualo, CropSoilWaterGoal: real);
var
  PETo, ET_Actualo, K_PlantEto, WaterShortage, WeekRain            : real;
  Day                                                              : Integer;
begin
PETo{poential ET, mm} := K_PanEt * EP_panWk;
```

[1] MOM source code of the knowledge part. Others see Appendix B.

```
K_PlantEto := 0.45 * LAI_Actualo; {LAI_Actualo <= 1.0}
if (LAI_Actualo > 1.0) and (LAI_Actualo <= 4.0) then
   K_PlantEto := 0.325 + 0.125 * LAI_Actualo;
if (LAI_Actualo > 4.0) then K_PlantEto := 0.85;
ET_Actualo{mm} := (K_PlantEto + K_SoilEt) * PETo;
if ET_Actualo < 0.0 then
   Form1.Memo1.Lines.Add(Format('ET Error %8.3f in Week %3d ', [ET_Actualo,
PresentWeek]));
WaterShortage := 0.0;
WeekRain := 0.0;
for L := 1 to TotalLayerNum - 1 do  {only count root zone}
  {The goal of soil moisture is 90-100% of Drain Limit}
  WaterShortage{mm} := 10.0 * (CropSoilWaterGoal * Water_DrainLmt[L] -
       Water_Actual[L]) * LayerThick[L];
for Day := 1 to TimeStep do WeekRain := WeekRain + DailyRainfall[Day];
WaterNeeded[PresentWeek] := WaterShortage + ET_Actualo - WeekRain;
if WaterNeeded[PresentWeek] < 0.0 then WaterNeeded[PresentWeek] := 0.0;
end;
```

2. Simulator

```
{ *******************   SoilWaterN_Simulation   ****************** }
Procedure SoilWaterN_Simulation(SimulationMode: TSimulateModes;
                                Lp_IrrgRate, Lp_FertRate, Lp_ChemIrrg : Integer);
{Before call this procedure, Must assign
    FertAmt[1..GrowWeek] by calling ReadFertScheduleCombinations(Lp_FertDate);
    DailyIrrgFraction[1..7] by calling ReadIrrgFreqCombinations(Lp_IrrgDate);}
var
  Day                                                            : Integer;

{-----  WaterProcesses  -----}
  ET_panDaily, LAI_Today, LAI_b, LAI_LastPeriod, TodayIrrg,
  Infiltration_Today                                             : real;

{-----  NitrogenProcesses  -----}
  N_UptakeCurveInLastDay, N_PlantDemand{kg/ha}, X, RootDepth_Last, {Normal}
  N_WeekPlantDemand, Demand_K, Fert_Eff{DetectN}, TodayFert       : real;

  label NoFertDaily, RainFeedCropping;

begin {*************   SoilWaterN_Simulation   ********************}

InitializationOfPlantGrowth;
Form1.Table3.First;   {First day: Rainfall and FertApp code data}
Demand_K := StrToFloat(Form1.EditDemandK.Text);          {for detect N}
Fert_Eff := StrToFloat(Form1.EditFertEff.Text);          { " }
if (SimulationMode = PredictGrowth) or (SimulationMode = Validation) then
   Form1.DBGrid1.Visible := true;

THISWEEK    := Form1.TodayDays div TimeStep + 1;
PresentWeek := 1;                              {default TimeStep is a week}
repeat          {  << = << ========  A growth season loop  =========  << = <<  }

Application.ProcessMessages;
N_InSoil_LastDay := N_TotalInSoil;      {Sum of N in soil layers}
SoilTemperature;                        {Air temp -> soil temp}
{if AirTempMax < 1.0 or SnowOccur then SnowFall procedure;}

{ ======  Initialization for daily loop  ======= }
ReadRainfallIrrigationFertCodeForAWeek;    {read from DB}

{--  Water portion  --}
DrainOutRootZone{cm} := 0.0;
ActualET_mm := 0.0;
Water_LastTotal :=0.0;
Infiltration := 0.0;
for L := 1 to TotalLayerNum do
  Water_LastTotal := Water_LastTotal + Water_Actual[L] * LayerThick[L];
```

```
{Set LAI and ET to daily}
if PresentWeek > 1 then LAI_LastPeriod := LAI_Curve[PresentWeek - 1]
  else LAI_LastPeriod := 0.0;
LAI_b := (LAI_Curve[PresentWeek] - LAI_LastPeriod)/TimeStep;
ET_panDaily := ETpan[PresentWeek] / TimeStep;

if (SimulationMode = DetectWater) and (PresentWeek >= THISWEEK) then begin
  {To determine Water Needed for this week}
  LAI_Today := (LAI_LastPeriod + LAI_b * 3.5) * LAI_Max;  {day = 3.5 : medium of week}
  EstimateWaterNeededThisWeek(ETpan[PresentWeek], LAI_Today, SoilWaterGoal);
  end;

{--  Nitrogen portion  --}
{Initialize SUM variables for N balance check later}
N_UptakePresentSum     := 0.0;
N_N2OPresentSum        := 0.0;
N_LeachedPresentSum    := 0.0;
N_FertilizerPresentSum := 0.0;
N_VoltPresentSum       := 0.0;
N_FoliarPresentSum     := 0.0;

{Plant uptake initialization}
if PresentWeek > 1 then N_UptakeCurveInLastDay := N_UptakeCurve[PresentWeek - 1]
  else N_UptakeCurveInLastDay := 0.0;
N_WeekPlantDemand := (N_UptakeCurve[PresentWeek] - N_UptakeCurveInLastDay) *
N_UptakeMax{kg/ha};
if N_WeekPlantDemand < 0.0 then N_WeekPlantDemand := 0.0;
N_PlantDemand := N_WeekPlantDemand / TimeStep;

if PresentWeek > 1 then RootDepth_Last := Root_Curve[PresentWeek - 1]
  else RootDepth_Last := 0.0;
RootIncrease := RootDepth_Max * (Root_Curve[PresentWeek] - RootDepth_Last)/TimeStep;
if RootIncrease < 0.0 then RootIncrease := 0.0;
for L := 1 to TotalLayerNum do N_Uptake[L] := 0.0;          {debug trace only}

if (SimulationMode = DetectN) and (PresentWeek >= THISWEEK) and
       (PresentWeek > 1) then begin {DetectN}
  {Add defficiency N detected last week to soil}
  Day := PresentWeek - 1;
  if N_Needed[Day] > 0.0 then begin
    N_FertilizerPresentSum{kgN/ha} := N_Needed[Day]{kg/ha};
    N_NH4_kgha[1] := N_NH4_kgha[1] + 0.5 * N_Needed[Day];
    N_NO3_kgha[1] := N_NO3_kgha[1] + 0.5 * N_Needed[Day];
    end;
  end; {DetectN}

Day := 1;                                            {  Day = 1..7 in a week    }
repeat                  {  <<  =========  Daily simulation loop  =========  <<  }
GrowthDay := GrowthDay + 1; {GrowthDay = 1... in a grow season}

{ ==========  Water movement and N leaching/upflow  =========== }
if Form1.ChkBoxRainFeed.Checked or (SimulationMode = Background) then begin
  Infiltration_Today := DailyRainfall[Day];
  goto RainFeedCropping;
  end;

if GrowthDay < Form1.TodayDays then TodayIrrg := DailyIrrigated[Day] {water applied
past}
  else { Water combinations in future}
    case SimulationMode of
      DetectWater,
      DetectN     : TodayIrrg := DailyIrrgFraction[Day] * WaterNeeded[PresentWeek];
      Optimization,
      PredictGrowth  : TodayIrrg := DailyIrrgFraction[Day] * PercentIrrg[Lp_IrrgRate] *
IrrgAmt[PresentWeek - 1];
      end; {case of}
Infiltration_Today := DailyRainfall[Day] + TodayIrrg;
if TodayIrrg > 0.0 then begin
  IrrgTimes := IrrgTimes + 1;            {accoount for labor cost}
  TotIrrgAmt := TotIrrgAmt + TodayIrrg;   {accoount for water cost}
  end;
```

```
if (WstApplied[Day] > 0) and Form1.ChkBoxWstIrrg.Checked then
  UpdateWasteFertilizerIrrigation(WstApplied[Day], TodayIrrg);

RainFeedCropping:  X := 0; {noting}

if Infiltration_Today > 0.0 then begin
  X := RunOff_Today(Infiltration_Today);
  RunOff_Total := RunOff_Total + X;  {mm}
  RunOff_Out   := RunOff_Out   + X;
  Infiltration_Today := Infiltration_Today - X;
  WaterIn := WaterIn + Infiltration_Today;
  end;
Infiltration_Redistribution(Infiltration_Today);
LAI_Today := (LAI_LastPeriod + LAI_b * Day) * LAI_Max;
if SimulationMode = DetectWater then N_ActualUptakeRate := 1.0; {assume no N uptake
problems}
Evapotranspiration(ET_panDaily, LAI_Today);

{MatricPotentialFlow;   Not significant: total amount < 1 cm usually}

{  ==========  N fertilization and transformation  ==============  }
if (SimulationMode = DetectWater) or (SimulationMode = Background) then goto
NoFertDaily;

if GrowthDay >= Form1.TodayDays then begin {Schdule in future}
  if (SimulationMode = DetectN) or (SimulationMode = Validation) then goto NoFertDaily;
  {Modes of Optimization, PredictGrowth  here}
  if FertAmt[PresentWeek - 1] <= 0.0 then goto NoFertDaily;
  if (Lp_ChemIrrg > 0) and (IrrgAmt[PresentWeek - 1] > 0.0) then begin
    {Add fertilizers with Irrg if irrigation schduled this week}
    X := DailyIrrgFraction[Day];
    if X > 0.0 then FertIrrgTimes := FertIrrgTimes + 1;
    end {Irrg Fert}
    else begin {Dry fertilization}
      X := DailyFertFraction[Day];
      if X > 0.0 then FertAppTimes := FertAppTimes + 1;
      end; {Dry fert}
  TodayFert := X * PercentFert[Lp_FertRate]*FertAmt[PresentWeek - 1];
  N_FertilizerPresentSum{kgN/ha} := N_FertilizerPresentSum + TodayFert;
  FertilizerIn := FertilizerIn + TodayFert;
  N_NH4_kgha[1]  := N_NH4_kgha[1]  + Fert_NH4  * TodayFert;
  N_NO3_kgha[1]  := N_NO3_kgha[1]  + Fert_NO3  * TodayFert;
  N_Urea_kgha[1] := N_Urea_kgha[1] + Fert_Urea * TodayFert;
  if (Fert_NH4 > 0.0) or (Fert_Urea > 0.0) then VolatizeDay := 0;
  if Fert_Urea > 0.0 then begin
    UreaHydrolDay := 0;
    UreaExist := True;
    end;
  end  {Schdule in future}
  else {applied past}
    if Fertilized[Day] > 0 then UpdateFertilizerApplication(Fertilized[Day],
LAI_Today);

NoFertDaily:

UpdateUreaHydrolyzeAndAnimalManureDecay(Day);
if VolatizeDay < 10 then AmmoniaVolatiliztion;   {NH3 start to volatilize}

{Nitrogen transformation in soil}
for L := 1 to TotalLayerNum do begin
  UreaHydrolysis;
  Mineralization_Immobilization;
  Nitrification;
  Denitrafication;
  end;

{Nitrogen uptake by plant}
if SimulationMode = DetectWater then RootDistribution(RootIncrease) {Assume N uptake
ok}
  else PlantNitrogenUptake(N_PlantDemand);
```

```
{ ======= Simulation output ======== }
case SimulationMode of
  PredictGrowth, Background,
  Validation  :  if SimulationOutput[Day] > 0 then GrowthSeasonOutput;
  end;

Day := Day + 1;
until (Day > TimeStep);      {  >>  ======  Daily simulation loop  ======  >>  }

if (SimulationMode = DetectN) and (PresentWeek >= THISWEEK) then begin
  {Determine N_Needed for this week, but add it in beginning of next week}
  N_Needed[PresentWeek] := (Demand_K * N_WeekPlantDemand -
N_UptakePresentSum)/Fert_Eff;
  if N_Needed[PresentWeek] < 0.0 then N_Needed[PresentWeek] := 0.0;
  {1/Fert_Eff = 0.26 - 2.46 * Log(Uptake Capacity)
   see TForm1.EditCropUptakeCapacityKeyDown(Sender:..)}
  end;

if WaterBalanceError > 0.00001 then Form1.Memo1.Lines.Add
       ('Water disbalanced = ' + format('%9.4g',[WaterBalanceError]));
if N_BalanceError > 0.00001{kg/ha} then Form1.Memo1.Lines.Add
       ('N disbalanced = ' + format('%9.4g',[N_BalanceError]));
N_TotalFertilizer := N_TotalFertilizer + N_FertilizerPresentSum;

Form1.GaugeCropGrow.Progress := round (100 * PresentWeek / TotalGrowWeek);
PresentWeek := PresentWeek + 1;
until (PresentWeek > TotalGrowWeek); { >> = >> ==  A growth season loop  == >> = >>  }
Form1.GaugeCropGrow.Progress := 0;
Form1.DBGrid1.Visible := False;

end;       { *******************   SoilWaterN_Simulation   ****************** }
```

3. Evaluator

```
Procedure SearchOptimalSolutions(AutoOpt: Boolean);
var
  I, J, SameLvlNodes, FertIncre, WaterIncre      : Integer;
  ProfitWt, YieldWt, LeachWt, GoalLimit, X        : real;
  Sect                                            : string;

  DistanceToGoal                                  : array[1..MaxNodes] of real;
{Sort nodes}
  GoalOrder                                       : array[1..MaxNodes] of Integer;
  Xuni                                            : array[1..3] of real;
  SchdFactor                                      : array[0..4] of Integer;
  IrrgDate, FertDate, NextFert, NextIrrg, NextX : array[0..MaxCombinations] of real;

  label NoSearch;

begin   {Tactiacl search}
if not Form1.StringGridSolution.Enabled then goto NoSearch;   {no nodes loaded}
if TotalSolution <= SharedNodes then goto NoSearch;           {too few nodes}

{Goal weights}
ProfitWt := 0.01 * FormMultDlg.ScrBarWeightProfit.Position;
YieldWt  := 0.01 * FormMultDlg.ScrBarWeightYield.Position;
LeachWt  := 0.01 * FormMultDlg.ScrBarWeightLeach.Position;
X := ProfitWt + YieldWt + LeachWt;
ProfitWt := ProfitWt / X;
YieldWt  := YieldWt  / X;
LeachWt  := LeachWt  / X;

{Dwt: relative weighted distance from current nodes to the goal.}
for I := 1 to TotalSolution do begin
  for J := 1 to 3 do begin
    {unify the varibles}
    if (GoalNodeMax[J, 0] - GoalNodeMin[J, 0]) < 1.0 then Xuni[J] := 1.0
      else begin
        X := TextToReal(Form1.StringGridSolution.Rows[I][10+J]);
```

```
        Xuni[J] := (X - GoalNodeMin[J, 0])/(GoalNodeMax[J, 0] - GoalNodeMin[J, 0]);
        end;                                        {EQ 5-3.7, 5-3.8, 5-3.9}
    end;
  X := ProfitWt * Xuni[1] + YieldWt * Xuni[2] + LeachWt * (1.0 - Xuni[3]);
  if X > 0.0 then DistanceToGoal[I] := 1.0 / FactorZeroToUnity(X) - 1
    else DistanceToGoal[I] := 1E10;
  GoalOrder[I] := I;
  end;

{Tactical search: Sort nodes by their DistanceToGoal, Dwt: Min -> Max }
for J := 1 to TotalSolution - 1 do begin
  for I := 1 to TotalSolution - J do
    if DistanceToGoal[I] > DistanceToGoal[I+1] then begin
      X                   := DistanceToGoal[I];
      DistanceToGoal[I]   := DistanceToGoal[I+1];
      DistanceToGoal[I+1] := X;
      L                   := GoalOrder[I];
      GoalOrder[I]        := GoalOrder[I+1];
      GoalOrder[I+1]      := L;
      end;
  end;

{Display the solution list, search nodes}
with Form1.StringGridSolution do begin
  for I := 1 to TotalSolution do begin
    for J := 1 to 8 do Rows[I][J] := Rows[GoalOrder[I]][J+10];
    Rows[I][J+1] := Format('%10.4g', [DistanceToGoal[I]]);
    end;
  ColCount := J + 2;
  end;

Order_OptimalSolution := 1;
if not AutoOpt then OutputSelectedNodeSchedule(Order_OptimalSolution);
        {Show first optimal Fert Water schedules}

{ ---------------  SuggestionForNextSimulations Start ---------------------------}
GoalLimit := DistanceToGoal[1]/(1.001 - FactorZeroToUnity(SharedERR));

{Find the number of the promising nodes that may share the same paths}
for I := 1 to TotalSolution do if DistanceToGoal[I] > GoalLimit then Break;
SameLvlNodes := I;
if SameLvlNodes > TotalSolution then SameLvlNodes := TotalSolution;
if SameLvlNodes < SharedNodes then SameLvlNodes := SharedNodes;

{Determine if having nodes that share the same rate level}
with Form1.StringGridSolution do begin
  for J := 0 to 4 do begin
    SchdFactor[J] := StrToInt(Rows[1][J+4]);
    for I := 2 to SameLvlNodes do
      {if the follows has different number, it is not shared, assign -1}
      if ABS(StrToInt(Rows[I][J+4]) - SchdFactor[J]) > 0.1 then SchdFactor[J] := -1;
    end;
  end;

{Read # of Dates series}
for I := 0 to mxLp_FertDate do
FertDate[I] := SumOfNonZeroMemberOfCol(TotalGrowWeek, I+2,
        Form1.StringGridWeeklyRate, X); {FertDate}
for I := 0 to mxLp_IrrgDate do
IrrgDate[I] := SumOfNonZeroMemberOfCol(TimeStep, I+2,
Form1.StringGridDailyFertIrrgFraction, X); {IrrgDate}

{Judg directions for the next simulation}
MOM_Ini := TIniFile.Create('MOM.ini');
try
with MOM_Ini do begin
  Sect := 'MOM Search';
  Form1.MemoSuggest.Clear;
  Form1.MemoSuggest.Lines.Add(Format('Upon first %3d nodes, suggests:',
[SameLvlNodes]));
  Form1.MemoSuggest.Lines.Add('');
```

```
  FertIncre := -9;
  WaterIncre := -9;
  if SchdFactor[0] >= 0 then X :=
NextSimulationDirection(ReadString(Sect,'FertTime','FertTime'),
                                FertDate, NextX, SchdFactor[0], mxLp_FertDate);
  if SchdFactor[1] >= 0 then FertIncre :=
NextSimulationDirection(ReadString(Sect,'FertRate','ThisFertRate'),
                                ThisFertRate, NextFert, SchdFactor[1], mxLp_FertRate);
  if SchdFactor[2] >= 0 then X :=
NextSimulationDirection(ReadString(Sect,'IrrgTime','IrrgTime'),
                                IrrgDate, NextX, SchdFactor[2], mxLp_IrrgDate);
  if SchdFactor[3] >= 0 then WaterIncre :=
NextSimulationDirection(ReadString(Sect,'IrrgRate','IrrgRate'),
                                ThisIrrgRate, NextIrrg, SchdFactor[3], mxLp_IrrgRate);
  if Form1.ChkBoxChemFert_Irrg.Checked then with Form1.MemoSuggest.Lines do
  if SchdFactor[4] > 0 then Add(ReadString(Sect,'FertIrrgOK','FertIrrgOK'))
    else Add(ReadString(Sect,'FertIrrgNo','FertIrrgNo'));
  end;
finally
  MOM_Ini.Free;
end; {try}

if AutoOpt then with Form1.StringGridRateChanges do begin
  {Change the rates for next MOM simulation}
  if FertIncre > -2 then
  for I := 0 to mxLp_FertRate do Rows[I+1][1] := Format('%8.4f', [NextFert[I]]);
{FertRate}
  if WaterIncre > -2 then
  for I := 0 to mxLp_IrrgRate do Rows[I+1][2] := Format('%8.4f', [NextIrrg[I]]);
{IrrgRate}
  end;

{ --------------  SuggestionForNextSimulations End -------------------------}

NoSearch : {nothing};

end; {SearchOptimalSolutions}


function NextSimulationDirection(S: String; var CurrentRate, NextRateTime :
       array of real; I_next, mxLoop : Integer): Integer;
var
  NextLvl                  : array[0..MaxCombinations] of real;
  Min, Max                 : real;
  I, I_min, I_max, Xsign   : Integer;
  label NoRange;

begin
  Min := CurrentRate[0];
  Max := Min;
  Xsign := -9;
  for I := 0 to mxLoop do begin
    NextRateTime[I] := 0.0;
    if CurrentRate[I] > Max then Max := CurrentRate[I];
    if CurrentRate[I] < Min then Min := CurrentRate[I];
    end;
if Max <= Min then Form1.MemoSuggest.Lines.Add('Range of rate or timing not found.');
if Max <= Min then goto NoRange;

{ ---------------  Suggest Start ---------------------------}
with Form1.MemoSuggest.Lines do begin
  if CurrentRate[I_next] >= Max then begin
    Add(S + ' -> Increase.');
    Xsign := 1;
    end;
  if CurrentRate[I_next] <= Min then begin
    Add(S + ' -> Decrease.');
    Xsign := -1;
    end;
  if (CurrentRate[I_next] > Min) and (CurrentRate[I_next] < Max) then
       Add(S + ' may be OK.');
```

```
  end;

  if Xsign > -2 then begin {assign changes}
    NextLvl[0] := CurrentRate[I_next];
    NextRateTime[0] := CurrentRate[I_next];
    for I := 1 to mxLoop do begin
      NextLvl[I] := NextLvl[I - 1] + Xsign * ChangeFraction;
      if NextLvl[I] < 0.0 then NextLvl[I] := 0.0;
      NextRateTime[I] := NextLvl[I];
      end;
    if  NextLvl[0] > NextLvl[mxLoop] then
      for I := 0 to mxLoop do NextRateTime[I] := NextLvl[mxLoop - I];
    end; {assign changes}
{ ----------------  Suggest End ----------------------------}
NoRange : {nothing}

Result := Xsign;

end; {NextSimulationDirection}
```

Appendix B

Software and Datasets

MOM software prototype with the source code are available from

MengBo LI,	mli@Hawaii.edu
	http://www2.hawaii.edu/~mli/
R.S. Yost,	rsyost@Hawaii.edu
	http://agrss.sherman.hawaii.edu/staff/yost.htm

or from the MOM Web:

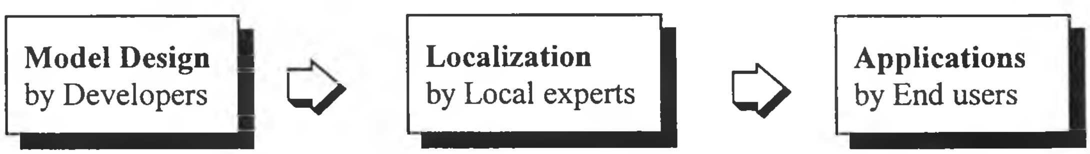
http://agrss.sherman.hawaii.edu/staff/MOM.html

The model scenarios are available from above sources. The validation datasets, however, are available based on permits from original dataset providers.

Appendix C

Localization of MOM

One of the greatest challenges to the N models designed in this study and other agricultural software is their adaptation to local conditions and to solving local problems. Unlike a commercial word processor software that can be simply installed and run anywhere, agricultural software must reflect local conditions. MOM must be adapted to reflect local conditions during installation processes by local extension agents or agricultural experts. The installation of agricultural software to local areas can be called Localization:



The localization process adapts or "trains" the models for specific agricultural areas or sites. Model performance depends on, in part, how well they are adjusted to local experience by local experts. The MOM parameters can be estimated from the calibration of local experiments but expensive. So local experts may estimate the parameters for MOM from literature or local knowledge.

Glossary

Some AI terms used in MOM are briefly described below to help readers understand the MOM processes. For more information, refers to Winston (1992).

Best-first search A heuristically informed search method. In best-first search, forward motion is from the best open node so far, no matter where that node is in the partially developed tree which may not direct to the global goal. However, the paths found by best-first search are likely to be shorter than those found by other methods, because best-first search always moves forward from the node that seems closest to the goal node.

Hill-climbing search A heuristically informed search method. Hill-climbing search uses a natural measurement of distance from each place to the goal to determine the move without examining all possible paths. In hill-climbing search, new paths are added into the search tree for further searches, based on estimated distances between their nodes and the goal.

Node A management strategy (or choice) combined with rates and timing of fertilization and irrigation.

Node state The results of profit, crop yield and leached nitrate that a node (management strategy) would produce in the model simulation. A node state is visually denoted by its positions in a space with dimensions of Y-axis against X-axis. Y-axis or X-axis can be either profit, yield, or leached nitrate. It is also called a **state space**.

Path A relation, or connection (visual link) between nodes, which represent the search (evaluation) moves from one node to another following some roles.

Search A process that evaluates nodes (management strategies). The search will lead to finding better nodes that would have higher profits and/or higher yields with lower nitrate leaching than other nodes.

Semantic net A node-and-link description that represents management strategies and their relations. The node-and-link net is also a **search tree** where the search moves from one node to another.

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