

Development and Preliminary Evaluation of the Simulation Model C-Maize VT1.0

by

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(ABSTRACT)

C-Maize VT1.0 is a simulation model of corn (*Zea mays*) growth in a soil-plant-atmosphere continuum. The purpose of developing the C-Maize VT1.0 simulation model was to provide an additional tool to researchers investigating the effects of water and nitrogen stress on corn growth and the movement of water and nitrates in the soil. The user may select either a 1-dimensional or a 2-dimensional approach to the simulation of the soil system. After an initial series of runs and a preliminary assessment of the model's credibility it was concluded that the 2-dimensional approach provided a 'sufficiently credible' solution to modeling all aspects of the soil-plant-atmosphere system. The 1-dimensional approach as currently programmed provides a 'non-credible solution'. The 1-dimensional approach failed to adequately simulate the soil subsystem and failed to simulate the plant's response to water and nitrogen stresses.

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Chapter 1: Development of the simulation model

C-Maize VT1.0

Introduction

C-Maize VT1.0 Simulation Model

C-Maize VT1.0 is a research level simulation model of corn (*Zea mays*) growth and development within a soil, plant, atmosphere continuum which includes both a 1-dimensional (1-D) and a 2-dimensional (2-D) approach to the simulation of the soil subsystem. The purpose of developing C-Maize VT1.0 was to provide an additional tool to researchers investigating the effects of water and nitrogen stress on corn growth and the movement of water and nitrates in soils. In the early stages of the model's development it was concluded that adequate models had already been developed to 1) describe corn growth and development and 2) model the soil subsystem following a 2-dimensional approach. It was decided that base models, which provided the basic system definitions, could be combined to meet the desired system definition.

Three criteria were used in the selection of the base models. First, the models selected should be adequately documented. Second, the corn model should be based on the phenologic and physiologic development of a corn plant. Finally, the models had to have been validated with actual field experiments. The crop model selected as the base model for corn growth and development was the nitrogen version of CERES-Maize (Jones and Kiniry, 1986). The soil subsystem model

selected was the RHIZOS portion of the cotton simulation model GOSSYM (Baker et al, 1983). Both models have been extensively rewritten and modified within the C-Maize VT1.0 system definition.

C-Maize VT1.0 runs under either version 1 or version 2 of Fortran 77. Complete documentation of the C-Maize VT1.0 simulation model is currently in preparation and will include both a User's Guide and a Programmer's Guide.

General System Theory

In order to adequately understand the C-Maize system a basic understanding of general system theory is necessary. Bertalanffy (1968) discusses general system theory in great detail. Some basic concepts are presented below.

The purpose of general system theory is to describe the principle concepts common to all systems. A system is defined as a collection of interacting elements or forces which operate to achieve a specific purpose. The study of systems in the sciences developed as science advanced from the study of the parts of a system to the study of parts in relation to the whole system.

Systems are generally defined at the two extremes as closed or open. A closed system is an isolated system which receives no stimulus from an outside environment and which tends toward a state of equilibrium or most probable distribution. An open system is any system which responds to continuous stimulus from an outside environment and produces an end result. In an open system, processes are described in terms of stimulus, response and feedback operating on or within the system. Figure 1, adapted from Bertalanffy (1968) outlines, in general terms, an open system.

One basic methodology for describing systems is the use of mathematics and logic. Mathematics are used to describe specific processes, interactions, and responses. The mathematical equations used to describe a system are characterized as either analytical or empirical. Analytical equations describe the physical processes under which a process, interaction, or response operates.

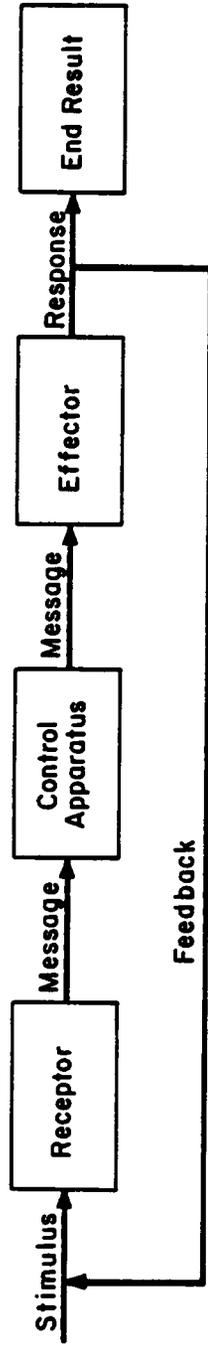


Figure 1. Open system definition (Bertalanffy, 1968)

Empirical equations describe the randomness associated with system processes, interactions or responses. Closed systems are normally described by analytic equations. Open systems are normally described by both analytic and empirical equations. Logic is used to describe the order and flow of system processes, interactions, and responses.

The use of mathematics and logic to describe systems is termed simulation modeling. Simulation models range from what are termed white box simulation models to black box simulation models (Karplus, 1983). White box models describe purely closed systems while black box models describe open systems empirically.

Most systems studied in the biological sciences when simulated are placed somewhere between the white box and black box models. The placement is highly dependent upon how the system is defined. Thus, the system definition is the most important aspect of simulation modeling.

Each system simulation model has properties of realism, precision, generality, and resolution. Realism refers to the theories and hypotheses used to describe the system. Precision refers to the ability of the model to faithfully predict the behavior of the system. Generality is the degree of simplification made about the system and the system's relationships. Resolution refers to the degree to which objects are included in the model and the time span over which the model will predict.

Given the above properties, simulation models are developed within a precise system definition, to meet specific objectives, and like statistics cannot be extrapolated beyond this definition. Even within the same system the balance of these properties shifts. How these properties are balanced is part of the system definition and reflect the purpose, economics, and prescribed use of the simulation model. For example, a research level simulation model will describe the processes, interactions, and response mechanisms associated with a system using as many analytical equations as possible to describe the systems processes, interactions, and response mechanisms. The same model, developed for a more general purpose, e.g. management, will use more empirical relationships to describe the processes, interactions, and response mechanisms than the research level model. Thus, the same system described under 2 different system definitions are not the same simulation model.

It is important to understand that simulation models are strictly tools in the study of systems. Simulation models, once defined and developed, provide tools with which to describe the behavior of a system, construct theories and hypotheses to describe observed behavior and/or use theories and hypotheses to predict the future behavior of a system. In simulation modeling the user experiments with the simulation model to obtain a specific result then, by changing one or more variables the user can draw quantitative conclusions about specific process effects on the simulated system, and from this draw qualitative conclusions about the affects on the real system. It is also important to understand that simulation models are evolutionary. Simulation models will evolve as basic and applied research develops new theories and hypotheses about a system and as computer technology develops faster and more advanced methods of problem solving.

Overview of C-Maize VT1.0 Mathematics and Logic

Model Objectives and Assumptions

The objective of C-Maize VT1.0 is to provide a tool to the researcher studying the effects of water and nitrogen stress on corn growth and water and nitrate movement under field conditions. C-Maize VT1.0 simulates the effects of water and nitrogen stress on corn growth, at a daily time step, within a soil-plant-atmosphere continuum and under a user prescribed management system. The C-Maize VT1.0 model consists of three interacting subsystems; the atmosphere, soil, and plant. The atmosphere subsystem supplies solar radiation, temperature, and rainfall to the plant and soil subsystems. The soil subsystem is that part of the system in which plant roots grow, which stores and releases water and nitrogen to the plant and outside environment, which redistributes water and nitrate-nitrogen within itself and which transforms nitrogen in organic sources to ammonium, from ammonium to nitrate and under saturated soil conditions from nitrate to gaseous forms of nitrogen. The plant is corn grown under cultivated conditions, at a defined population density, with predetermined phenotypic and physiologic characteristics. Corn growth is based on the ability of the corn plant to produce carbohydrates from the energy supplied by solar radiation. The carbohydrates produced may then be reduced by the inability of the soil to supply water or nitrogen re-

quired for the carbohydrate production and by extremes in atmospheric air temperatures, whichever is the most-limiting factor. These responses can be modified through irrigation, nitrogen fertilization and surface residue management practices. All other responses or management practices which theoretically affect field corn growth are not considered part of the system definition and should be considered non-limiting.

Modeling Approaches

Within C-Maize VT1.0 two separate modeling approaches are available to the user. These approaches represent two different hierarchical levels of modeling the soil system. The modeling approaches are referred to as a 1-dimensional (1-D) approach and a 2-dimensional (2-D) approach. The 1-D approach takes a more generalized approach to the soil subsystem definition than the 2-D approach. The 2 approaches differ in their calculation of a number of processes which occur within the soil subsystem.

1-Dimensional Approach to Soil Subsystem Processes

The 1-D approach follows, with modifications, the approach of the base model CERES-Maize (Jones and Kiniry, 1986). Following the 1-D approach, a corn plant is grown in a soil system with a maximum of 10 user defined layers extending to a depth of 200 cm or to an impermeable layer, whichever is least (Figure 2). Each layer is defined from user input in terms of available water contents.

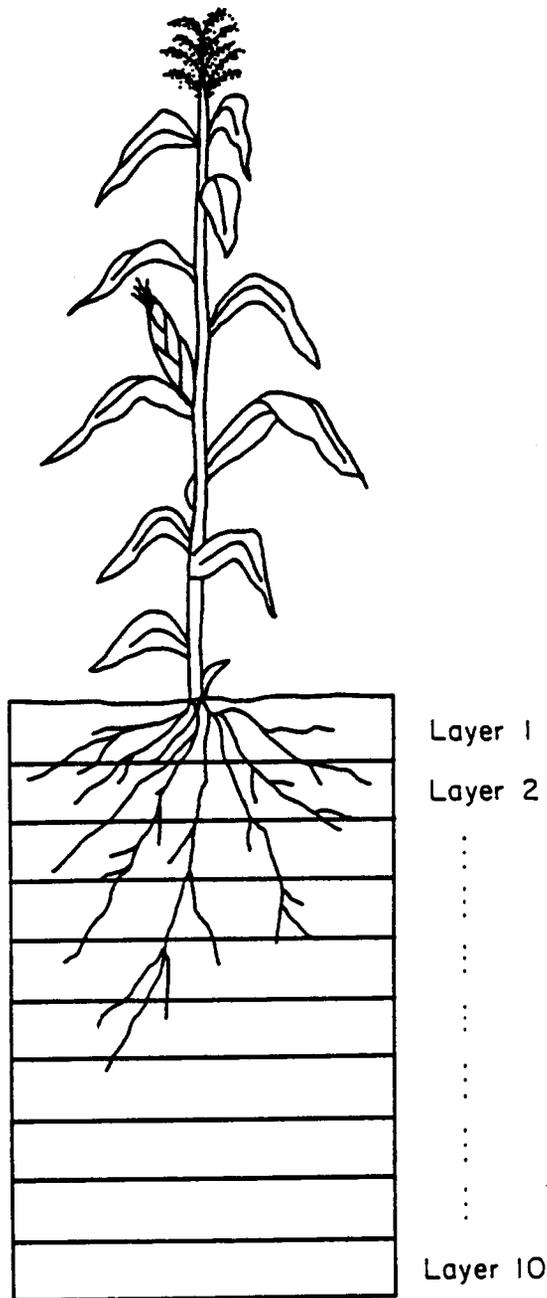


Figure 2. Model Conceptualization of 1-Dimensional Approach

2-Dimensional Approach to Soil Subsystem Processes

The 2-D approach is based on the conceptualizations of the RHIZOS portion of the cotton model GOSSYM (Baker et al., 1983). RHIZOS has been extensively modified in its incorporation into C-Maize VT1.0. Following the 2-D approach, the soil is modeled underneath a corn row, where the soil depth and inter-row spacing of the crop are partitioned by the user to form a grid matrix of equal sized grid cells (Figure 3). Each soil layer defined in the 2-D approach represents soil profile horizons of distinctly different soil water retention characteristics and are defined by user input (Molten et al., 1987a) in terms of the variables described by van Genuchten (1980).

Model definition

This section provides an overview of the processes, interactions, and response mechanisms included in the C-Maize VT1.0 model. Because there are 2 distinct modeling approaches available the user should be aware of the differences between the processes, interactions and response mechanisms of the two approaches as discussed in this section.

Management practices

The user describes, during input, the management system to be simulated. Included in this description are irrigation, nitrogen fertilization, and surface residue management practices.

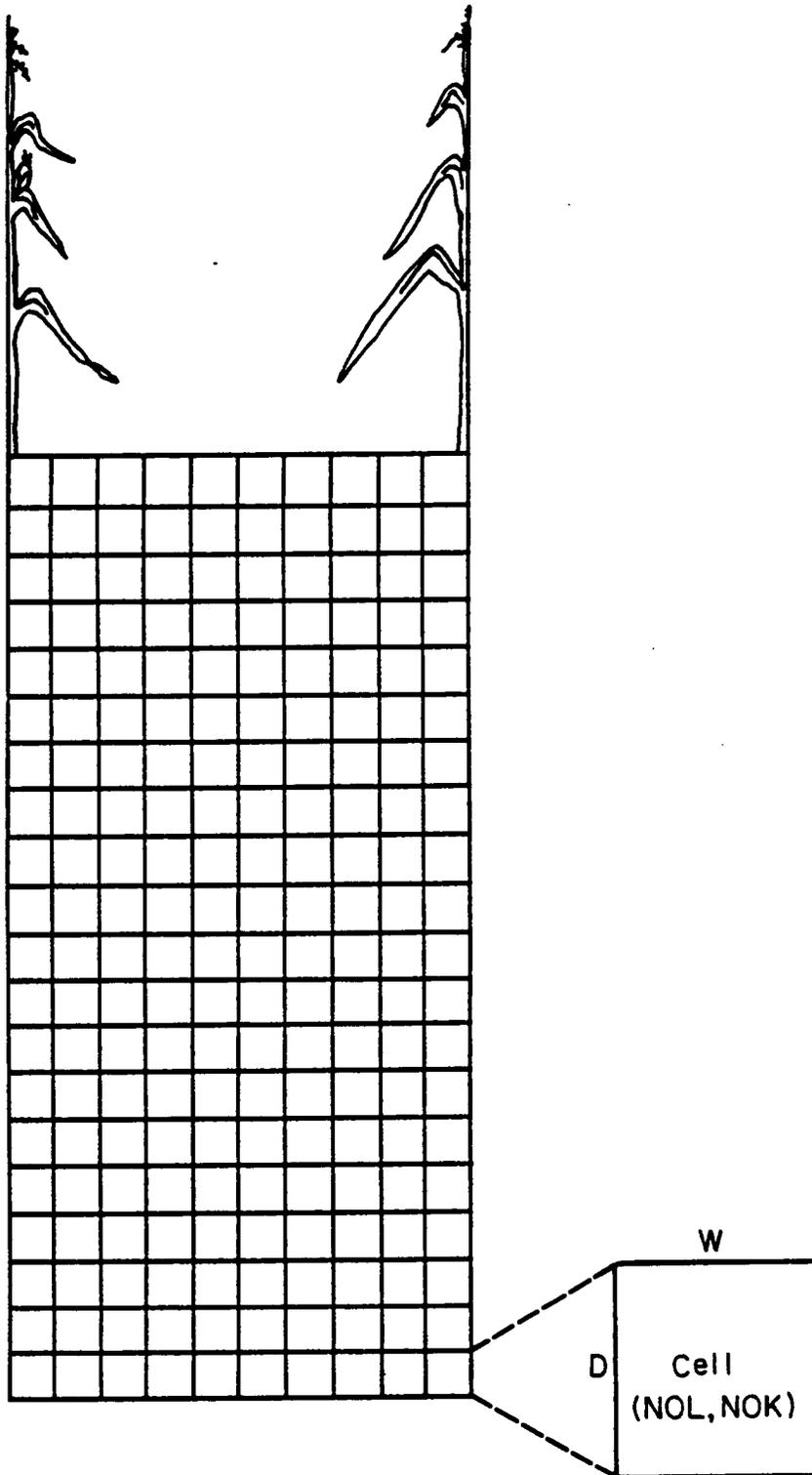


Figure 3. Model Conceptualization of 2-Dimensional Approach

Irrigation

Irrigation water can be added by the user through a specified schedule or the amount of water to be added can be automatically determined by the model. The user specifies at input either to apply irrigation from a schedule or to automatically apply water. The difference between the 2 modeling approaches is that the 1-D approach brings the entire soil profile to the drained upper limit of plant available water while the 2-D approach only brings the root zone to the drained upper limit.

Nitrogen fertilization.

Nitrogen fertilizer is added to the system as specified by the user. The user specifies the date, amount, and type of fertilizer to be applied and the method of application. Fertilizer can be surface applied or broadcast and incorporated under either modeling approach. The 2-D approach also allows for banding of nitrogen fertilizer.

Surface residue management

When modeling nitrogen the amount of organic matter remaining on the surface from a previous crop will affect the levels of nitrogen in the soil and the amount of water runoff. The user describes, during input, the initial amount and type of organic matter in the system, whether the organic matter is incorporated and an appropriate runoff curve number for the surface conditions.

Atmosphere Subsystem Processes and Interactions

The atmosphere subsystem supplies the stimuli to which the C-Maize system responds. The atmosphere subsystem consists of reading actual daily weather parameters as input. These parameters include solar radiation, maximum and minimum air temperatures, and rainfall amounts. This step also increments the daily time step within C-Maize. The atmosphere affects numerous soil and plant processes. The atmosphere affects soil temperature, soil surface evaporation, and advances the thermal time upon which the phenologic growth of the plant is based.

Heat units for phenologic development are accumulated as daily thermal units (DTT) at a base temperature (T_{base}) of either 10°C or 8°C. A base temperature of 10°C is used from germination to emergence. A base temperature of 8°C is used for the remaining growth stages. Daily thermal time (DTT) is calculated as

$$DTT = 0. \quad T_{max} < T_{base}$$

$$DTT = T_{mean} - T_{base} \quad T_{base} < T_{min} \leq T_{max} < 34$$

where T_{max} is the maximum daily temperature, T_{mean} is the mean daily temperature, and T_{min} is the minimum daily temperature. When the minimum temperature is less than the base temperature and/or the maximum temperature is greater than 34°C, the daily thermal time accumulated is calculated as the average thermal time accumulated over 8 3-hour intervals as

$$DTT = \frac{\sum_{n=1}^8 [T_{min} \times FAC_n \times (T_{max} - T_{min})]}{8}$$

where FAC_n is a thermal constant for each of the 8 3-hour periods.

The atmosphere also supplies the energy necessary for production of carbohydrates. This energy is supplied as solar radiation and carbohydrate production is based on that portion of the solar radiation received which is photosynthetically active. Photosynthetically active radiation

(PAR) is assumed to be 50 percent of the daily amount of solar radiation (SOLRAD) received and is calculated as

$$\text{PAR} = 0.02 \times \text{SOLRAD}$$

where the factor 0.02 includes both the conversion from langleys/d to MJ/d and the 50 percent reduction factor.

Potential evapotranspiration

Both models calculate potential evapotranspiration following the 2-stage drying process developed by Ritchie (1972). The 2 modeling approaches do not differ in the method of calculation of potential evapotranspiration.

Following Ritchie's (1972) approach, the evaporative flux (EEQ) of the crop surface is calculated as

$$\text{EEQ} = \text{SOLRAD} \times (2.04 \times 10^{-4} - 1.83 \times 10^{-4} \times \text{ALBEDO}) \times (\text{TD} + 29)$$

where ALBEDO is the cropping surface albedo and TD is the daily temperature adjusted for day length. The potential evapotranspiration (E0) is calculated by adjusting the surface evaporative flux for daily temperature. Soil evaporation (EOS) is calculated based on the leaf area index (LAI) of the crop

$$\text{EOS} = \text{E0}/1.1 \times \exp(-0.4 \times \text{LAI}) \quad \text{LAI} > 1.0$$

$$\text{EOS} = \text{E0} \times (1.0 - 0.43 \times \text{LAI}) \quad \text{LAI} \leq 1.0$$

The potential soil evaporation (ES) is then adjusted for the surface drying condition. Two surface drying conditions, stage-1 and stage-2, are described by Ritchie (1972) as affecting ES. Stage-1 drying indicates the surface is acting as a free water surface. Stage-1 drying occurs when the soil surface is saturated until a user defined limit (U) has been evaporated. Once this limit has been reached stage-2 drying occurs.

The potential plant evaporation (EP) is calculated based on the LAI of the crop

$$EP = E_0 \times (1.0 - \exp(-LAI)) \quad LAI \leq 3.0$$

$$EP = E_0 - ES \quad LAI > 3.0$$

where EP is not allowed to exceed the difference between E0 and ES.

Plant Subsystem Processes and Interactions

The plant subsystem is the effector in the system. The plant system is a corn crop which receives stimuli from the atmosphere and adjusts its response to the atmospheric stimuli based on the responses supplied through the soil subsystem. The atmosphere subsystem determines the transpirational demand, and the development and growth of the plant. Atmospheric air temperature is used as the stimulus for advancing plant growth through the phenologic growth stages. The atmosphere supplies solar radiation as a stimulus to the plant production of carbohydrate. Low moisture and nitrogen contents in the soil subsystem reduce the ability of the plant to produce carbohydrates. There is no difference between the model approaches with regard to either the phenologic or physiologic development of the plant. The phenologic and physiologic development of the corn plant are based upon the conceptualizations used in CERES-Maize (Jones and Kiniry, 1986) with minor modifications.

Phenologic development

Plant growth is dependent upon the growth stage of the plant. C-Maize VT1.0 uses 9 stages for advancing the plant through the growing season. Two of the growth stages are pre-growth and the remaining 7 represent the phenologic growth stages of corn. For ease of programming these stages are defined as:

7--Presowing.

8--Sowing to Germination.

9--Germination to Emergence.

1--Emergence to end of Juvenile Stage

2--End of Juvenile stage to Tassel Initiation.

3--Tassel initiation to end of leaf growth and silking.

4--Silking to beginning of grain fill

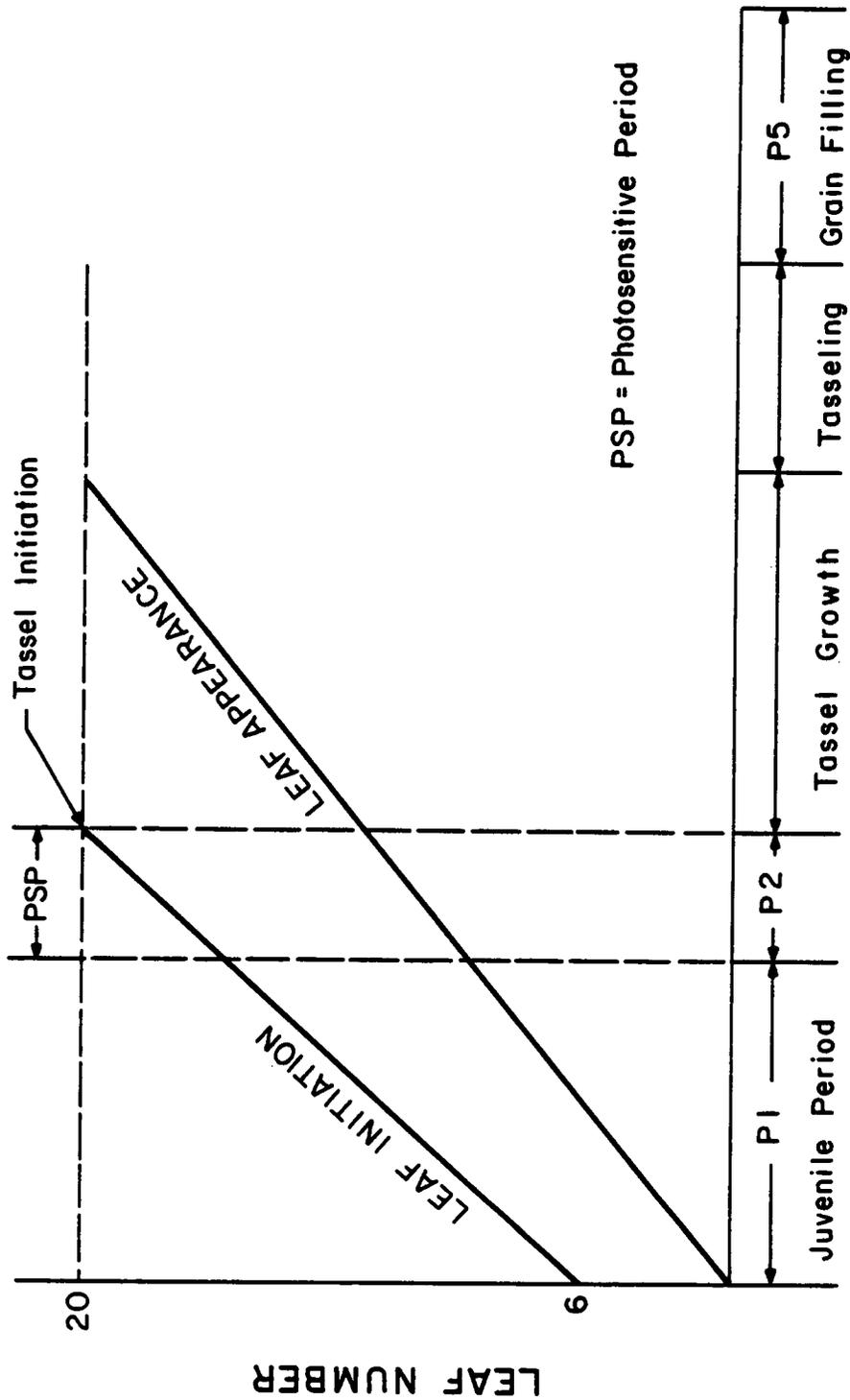
5--Effective grain filling period

6--End of grain filling period to Physiological maturity.

Figure 4 (T. Hodges, 1986, personal communication) represents how the corn plant is advanced phenologically through growth stages 1 through 5. Once the crop has been planted and germination has been determined thermal time accumulation determines the beginning and end of the growth stages. Each growth stage is initialized based on different characteristics and are therefore discussed individually below in order of advancement.

Advancement from growth stage 7 to growth stage 8

Each simulation begins at growth stage 7. Growth stage 8 is initialized on the date the crop is planted.



THERMAL TIME

Figure 4. Conceptualization of Corn Growth in C-Maize VT1.0 (T. Hodges, 1986, personal communication)

Advancement from growth stage 8 to growth stage 9.

Advancement from growth stage 8 to growth stage 9 is dependent upon the soil moisture status of the layer or cell in which the seed was planted. A soil water deficit factor affecting germination is calculated based on the soil moisture content of the layer or cell in which the seed is planted. Growth stage 9 is initialized on the first day the soil water deficit factor exceeds 0.02. If growth stage 8 exceeds 40 days in length, indicating germination has not occurred within 40 days, the crop fails and the growth stage is advanced immediately to growth stage 5.

Advancement from growth stage 9 to growth stage 1.

The plant advances from growth stage 9 to growth stage 1 when the accumulation of thermal time at a base temperature of 10°C exceeds the thermal time required for emergence (P9). The parameter P9 is calculated by the program based on the sowing depth of the crop.

Advancement from growth stage 1 to growth stage 2

The plant advances from growth stage 1 to growth stage 2 when the accumulation of thermal time at a base temperature of 8°C exceeds the parameter P1 specified as a crop genetic parameter by the user during input.

Advancement from growth stage 2 to growth stage 3

The plant advances from growth stage 2 to growth stage 3 when the photoperiod induction rate exceeds 1.0. The photoperiod induction rate is calculated based on the accumulation of thermal time and the parameter P2 specified as a crop genetic parameter by the user during input.

Advancement from growth stage 3 to growth stage 4

The plant advances from growth stage 3 to growth stage 4 when the accumulation of thermal time at a base temperature of 8°C exceeds the parameter P3. The parameter P3 is a crop genetic parameter calculated by the program. The value of P3 is dependent upon the total leaf number of the plant and the accumulated thermal time.

Advancement from growth stage 4 to growth stage 5

The plant advances from growth stage 4 to growth stage 5 when the accumulation of thermal time at a base temperature of 8°C exceeds 170.

Advancement from growth stage 5 to growth stage 6

The plant advances from growth stage 5 to growth stage 6 when the accumulation of thermal time at a base temperature of 8°C exceeds 95 percent of the parameter P5 specified as a crop genetic parameter by the user during input.

Determination of end of growth stage 6 and calculation of yield estimates

The plant determines the end of growth stage 6 and calculates the estimated yields when the accumulation of thermal time at a base temperature of 8°C exceeds the remaining 5 percent of the variable P5 specified as a crop genetic parameter by the user during input.

Physiologic growth

The physiologic growth of the plant once it has emerged is simulated as the potential carbohydrate produced by the plant as a function of the solar radiation supplied by the atmosphere and the leaf area index of the plant. The potential amount of carbohydrate produced is then reduced by temperature, soil water, and nitrogen response factors.

After the phenologic growth stage of the plant has been determined the potential carbohydrate production is calculated based on the photosynthetically active radiation and the leaf area index of the plant. The partitioning of carbohydrates to the actively growing plant parts is dependent upon the growth stage of the plant.

Once the amount of carbohydrate produced each day has been determined the number of leaves on the plant are calculated, if the plant is in vegetative development. Carbohydrate is then partitioned to the actively growing plant parts dependent upon the current phenologic growth stage of the plant.

Partitioning of Carbohydrates during growth stages 1 and 2

During growth stages 1 and 2, plant carbohydrate is partitioned to the leaves and roots. The carbohydrate distributed to the leaves is calculated as a function of the plant leaf area. The remaining carbohydrate is partitioned to the roots. During growth stage 1, preference for carbohydrates is given to the roots. When the roots receive less than 25 percent of the total carbohydrate fraction leaf weight increase is reduced to 75 percent of the total available carbohydrate and 25 percent is partitioned to the roots. During growth stage 2, preference for carbohydrates is given to the leaves. A minimum of 75 percent of the daily carbohydrate produced must be partitioned to the leaves.

Partitioning of carbohydrates during growth stage 3

During growth stage 3, carbohydrates are distributed to the stems, leaves, and roots of the plant. The partitioning of the carbohydrates to the leaves and stems is dependent upon the daily leaf area increase which is dependent on the number of leaves exposed and the soil water deficit factor affecting cell expansion. When less than 12 leaves are exposed, the leaf area increase is determined as a function of leaf number and the accumulation of daily phyllochron increments. Carbohydrate distribution to the leaf is determined as a function of the leaf area increase and the plant's total leaf area. Carbohydrate distribution to the stems is determined as a function of the daily leaf weight and total number of plant leaves. When the plant contains more than 12 leaves, but 3 less than the total maximum leaf number, the daily leaf area increase is calculated as a function of the daily phyllochron increments accumulated. Carbohydrates are distributed to the leaves as a function of the daily leaf area increase and the total plant leaf area. The carbohydrate distributed to the stems is again a function of the carbohydrate to be distributed to the leaves and the total leaf number. During the development of the last 3 leaves, the daily leaf area increase is calculated as a function of current leaf number, total leaf number, and the daily phyllochron units accumulated. Carbohydrate to be distributed to the leaves is calculated as a function of daily leaf area increase and total plant leaf area. However during this period carbohydrate supply for stem growth is determined as a function of daily phyllochron units accumulated.

The carbohydrate partitioned to the roots is the amount of carbohydrate remaining after leaf and stem growth. A minimum of 10 percent of the total available carbohydrate must be partitioned to the roots. When less than 10 percent of the available carbohydrate is supplied to the roots the carbohydrates partitioned to the leaves and stems are reduced proportionately in order to supply 10 percent of the daily increase in carbohydrate to the roots.

Partitioning of carbohydrates during growth stage 4

During growth stage 4, carbohydrates are partitioned to the ears, stems, and roots. Carbohydrate distribution to the ears is calculated as a function of daily thermal units and is reduced due

to low soil moisture contents. Carbohydrate available for stem growth is assumed to equal 40 percent of the carbohydrate available for ear growth. Carbohydrate supplied to the roots is the amount of carbohydrate not distributed to the ears or stems. If less than 8 percent of the daily carbohydrate is partitioned to the roots, then the carbohydrates supplied to the ears and stems are reduced proportionately so that a minimum of 8 percent of the daily carbohydrate is partitioned to the roots.

Partitioning of carbohydrates during growth stage 5

During growth stage 5, daily carbohydrates are partitioned to the grain, stems, and roots. Carbohydrate is partitioned to the grain as a function of the daily rate of grain fill, the number of grains per plant and the maximum rate of grain fill specified as crop genetic parameters by the user as input. The daily rate of grain fill is a function of the atmospheric air temperature and the maximum rate of grain fill is a parameter input by the user. If the daily rate of grain fill falls below 0.1 for two or more consecutive days the crop matures at its current state due to slow grain fill. Carbohydrate distribution to stems is 50 percent of any carbohydrate remaining after grain fill. The remaining 50 percent of the carbohydrate is partitioned to the roots. If grain growth requires all or more than the daily amount of carbohydrate produced no carbohydrates are partitioned to the stems or roots. All of the carbohydrate is partitioned to the grain and if additional amounts are still required to meet the daily demand up to 20 percent of the maximum stem weight is partitioned to the grain and the stem weight is reduced to reflect the loss. If additional amounts are still required up to 15 percent of the maximum leaf weight is partitioned to the grain and the leaf weight is reduced to reflect the loss.

Nitrogen partitioning to plant parts

The nitrogen taken up by the plant is partitioned to the plant parts depending on the growth stage of the plant and the modeling approach being used.

During growth stages 1 through 4 the nitrogen taken up is partitioned to the stover and roots of the plant. The method for partitioning nitrogen to the stover and roots during these growth stages is dependent on the modeling approach.

In the 1-D approach nitrogen is taken up to meet the demand of the plant. The amount of nitrogen taken up is partitioned to the stover and roots proportionate to the total demand of the individual plant parts.

In the 2-D approach the nitrogen demand of the stover and roots is assumed to be 4 percent of the total weight of these plant parts. Because excess nitrogen is allowed to be taken up by the plant under the 2-D approach the partitioning of the nitrogen is dependent upon whether or not the stover and roots demand are greater than 0 or equal to 0. When the demand of the stover and roots exceeds 0 the nitrogen taken up is partitioned proportionate to the demand of the individual parts. If however the demand equals 0 the nitrogen taken up is partitioned equally to the stover and roots.

In either the 1-D or the 2-D approach the nitrogen taken up during growth stage 5 is assumed to be taken up strictly to meet the grain demand for nitrogen. If excess nitrogen is taken up beyond the grain demand it is partitioned equally to the stover and roots of the plant. If, however, the grain nitrogen demand exceeds the amount taken up, the plant is allowed to transport nitrogen from the stover and the roots. Translocation of nitrogen is allowed from the stover when the stover contains greater than 4 percent nitrogen by weight. Translocation of nitrogen is allowed from the roots when the roots contain greater than 2 percent nitrogen by weight.

Soil Subsystem Processes and Interactions

The soil subsystem acts as both a receptor and as a response apparatus (Figure 1). As a receptor, the soil accepts stimuli from the atmosphere and the plant. Atmospheric stimuli affect soil temperature, soil evaporation and soil moisture contents. When nitrogen is also simulated the atmosphere stimulates the processes of mineralization and immobilization, nitrification, and denitrification. Plant stimuli include the root uptake of water and nitrogen from the soil which in turn stimulates the redistribution of water and nitrate-nitrogen within the soil. The soil subsystem acts as a response apparatus to the plant by reducing plant growth due to low soil water and nitrogen contents.

After the atmosphere subsystem has advanced the time step the soil subsystem is updated. The soil processes and interactions are updated depending on the modeling approach selected by the user. The processes and interactions used to update the soil system are discussed below and the differences between the approaches are described.

Soil temperature distribution

Soil temperature is updated in the soil system following the approach used in the EPIC model (Williams and Renard, 1985). Soil surface temperature is determined based on a 5-day running average surface temperature and is distributed with depth based on a damping factor for depth and the average soil moisture content of the profile. There are no differences in the calculation of soil temperature under either modeling approach.

The daily surface temperature (DT) is calculated as

$$DT = ST0 - (TAV + AMP \times \cos(ALX/2))$$

where ST_0 is the surface temperature of soil averaged over the past 5 days, TAV is the long term average temperature of the site, AMP is the annual amplitude of the mean monthly air temperature and ALX is the day of the year as a radian fraction of 1 year. The damping depth is calculated based on the average soil moisture content and bulk density of the soil profile. The soil temperature of each layer in the soil is then calculated as

$$ST_i = TAV + (AMP/2. \times \cos(ALX + DT) \times \exp(Z/DD)$$

where Z is the depth of the soil layer and DD is the damping depth.

Root weight distribution in soil subsystem

The distribution of root weights into the soil differ significantly between the modeling approaches.

In the 1-D approach, root carbohydrates are partitioned to each layer as

$$RLV_i = RLV_i + RLNEW \times \frac{WR_i}{TRW} \times \frac{RLDF_i}{TRLDF} - 0.005 \times RLV_i$$

where RLV_i is the current root length volume in a layer, $RLNEW$ is daily root length to be distributed, WR_i is a user assigned weighting function, TRW is the summation of the weighting factors for all layers contained in the root zone, $RLDF_i$ is a reduction factor for reducing root growth due to limiting soil water, nitrogen or soil temperature, $TRLDF$ is the sum of all reduction factors through the rooting depth, and 0.005 is the assumed fraction of roots sloughed each day. The total root depth of the plant is assumed to be a function of the daily thermal time adjusted for soil moisture conditions as

$$RTDEP = RTDEP + DTT \times 0.225 \times SWDF1$$

where DTT is the daily thermal time and SWDF1 is the soil moisture factor affecting plant growth.

In the 2-D approach, root growth follows the conceptualizations presented in the RHIZOS portion of the GOSSYM simulation model (Baker et al., 1983). Root weights are partitioned, in each cell containing roots, into 3 age classes. Class 1 roots are 1 to 3 days old. Class 2 roots are 4 to 12 days old. Class 3 roots are greater than 12 days old. These age classes are used to determine potential new root weight increases in each cell and the potential uptake of water and nitrate-nitrogen from each cell.

Potential root weight increase in each cell is increased as a fraction of the total root weight in the cell capable of growth. The total weight of class 1 roots is allowed to produce new root weights, 50 percent of the total weight of class 2 roots is allowed to produce new root weights and 20 percent of the total weight of class 3 roots is allowed to produce new root weights. The total root weight increase in each cell is fractionally reduced by low soil water contents, low total nitrogen contents or extremes in soil temperatures, whichever is the most limiting factor. The actual root weight increase in each cell is determined as a fraction of the carbohydrate supplied to the root system in proportion to the total potential root weight increase of the root system. It is assumed that the new dry weight increase in the root system is 70 percent of the carbohydrate partitioned to the root system, the remaining 30 percent is assumed lost to respiration. The new root weights are added to each cell and if the previous day's total root length exceeds the dimensions of the cell, the new root weights are partitioned to surrounding cells. Roots are not allowed to grow upward and a weighting factor for geotropism is employed to partition more roots to the cell immediately below the cell which initiated the root weights.

The root length in each cell is calculated from the equation:

$$L_r = \frac{4W_r}{\pi D d^2} \quad [1]$$

where L_r is the total root length in a cell, W_r is the total weight of roots in a cell, D is the density of roots, assumed to equal 1.0 g/cm^3 , and d is the average root diameter of the root system. Average root diameters are assumed to equal 0.02 cm during growth stage 1 and 2 and 0.04 cm during growth stages 3, 4, and 5.

The assumed average diameters of the root system were determined based on the work of Mengal and Barber (1974) who measured both root lengths and root weights of corn grown under field conditions in 1970 and 1971. From the data presented by Mengal and Barber (1974), high correlation coefficients were found between total root length and total root weight for plants 15 to 96 days old in 1970 ($R^2 = 0.987$) and 21 to 132 days old in 1971 ($R^2 = 0.901$). An overall correlation coefficient of 0.8981 was found when both years were combined.

By rearranging equation 1 and assuming a root density of 1.0 g/cm^3 the diameter of the root can be determined from the equation:

$$d = \left[\frac{4W_r}{\pi 1.0 L_r} \right]^{0.5}$$

Also by rearrangement and assuming an average root diameter of 0.04 cm over the growing season the average root density can be determined from the equation:

$$D = \frac{4W_r}{\pi L_r (0.04)^2}$$

Table 1 gives the average values for d and D , calculated from the above equations using the data presented by Mengal and Barber (1974).

Two regression analyses were performed on the data presented by Mengal and Barber (1974). The first analysis regressed L_r against $4W_r/\pi$ and the second regressed L_r against $4W_r/(\pi \times (0.04)^2)$. Both analyses assumed no y -intercept. The regression coefficient from these results are assumed

Table 1. Average root diameter (d) and root density (D) calculated from root weight and root length data of Mengal and Barber (1974)

Year	d (cm)	D g/cm ³
1970	0.038	1.001
1971	0.040	1.080
1970 & 1971	0.039	1.049

to equal $1/(Dd^2)$ and $1/D$ respectively. The regression coefficients could then be used to determine the mean root diameter as

$$d = [Dd^2/D]^{0.5}$$

The results of these analyses and calculations are presented in Table 2.

The variables D and d in Table 1 closely estimate the values in Table 2. All average values for D in Table 2 fall somewhat short of the assumed value of 1.0 g/cm^3 , while the values for D in table 1 are very close to 1.0 g/cm^3 especially in the year 1970. The lower values for the regressed value of D most probably include variation due to laboratory and field sampling. The 1970 data were taken when the corn plants were 15 to 96 days old. This represents more samples taken earlier in the season than in 1971 and also a shorter sampling period. Thus the 1970 data most probably represents younger roots as a whole than the 1971 data.

From the above analysis the assumption is made in the 2-D approach that the average corn root density equals 1.0 g/cm^3 through the entire growing season and that the average root diameter is 0.04 cm during growth stages 3, 4, and 5. An average root diameter of 0.02 cm is assumed during growth stages 1 and 2 to account for faster root elongation during the early growth stages of the corn plant.

The regression equations developed here pertain to the fresh weights of roots. The program assumes that the carbohydrate partitioned to the roots increases the dry weight of roots. A conversion factor for converting dry weight to fresh weight is needed for calculating root length. Root length is calculated as

$$RTLEN_c = \frac{4 \times (TRTS + 0.26 \times TRTS)}{(1.0 \times 3.1417 \times d^2)}$$

where $TRTS$ is the dry weight of roots, d is average root diameter, and 0.26 is the assumed average weight percent of water in the roots.

Table 2. Results of regression analysis from Mengal and Barber (1974)

Year	$1/Dd^2$ (cm/g)	Dd^2 (g/cm)	$1/D$ (cm ⁻¹)	D (g/cm ³)	R^2	d^* (cm)
1970	862.51	0.0012	2.272	0.440	0.9859	0.05
1971	1419.99	0.0007	1.380	0.725	0.9288	0.03
1970-71	932.24	0.0011	1.492	0.670	0.0985	0.04

* $d = (Dd^2/D)^{0.5}$

Mineralization and Immobilization

Calculation of the mineralization and immobilization of nitrogen from organic sources follows the approach used in PAPRAN (Seligman and van Keulen, 1981). Mineralization of the fresh organic matter in the soil is determined based on the decomposition rate of the carbohydrate, lignin, or cellulose fraction, whichever is currently decomposing, and on the carbon:nitrogen ratio of the fresh organic matter. The rate is also adjusted due to moisture and temperature stresses which would affect the growth of soil organisms. The stable organic, or humic, fraction is mineralized based on a constant rate of mineralization adjusted by the user for soil chemical and physical limitations. The model assumes that 2 percent of the nitrogen released from the fresh organic fraction is immobilized by the soil organisms. The model also assumes that 20 percent of the fresh organic nitrogen fraction is reduced to humus and thus 80 percent of the total amount released is actually mineralized. All nitrogen released from the stable organic fraction is added to the ammonium-nitrogen supply. There is no difference between the modeling approaches in the calculation of mineralization and immobilization.

Nitrification

The maximum daily nitrification rate is calculated under both approaches as a Michaelis-Menton first order reaction equation

$$V_{\text{NO}_3} = V_{\text{max}} \times \frac{[\text{NH}_4]}{K_{\text{NO}_3} + [\text{NH}_4]}$$

where V_{NO_3} is the maximum daily rate of nitrification, V_{max} is the maximum rate of nitrification, K_{NO_3} is the Michaelis Menton constant for nitrification and $[\text{NH}_4]$ is the ammonium-nitrogen concentration in the layer or cell. V_{max} is assumed to equal 40 Kg/(ha d) and K_{NO_3} is assumed to

equal 90 Kg/ha. The maximum daily rate of nitrification is then reduced by a reduction factor which is dependent on the modeling approach being used. In the 1-D approach 3 reduction factors are determined; a soil moisture reduction factor, a soil temperature reduction factor, and a nitrification capacity factor. The daily nitrification rate is reduced by the most limiting of these 3 factors. In the 2-D approach only the soil moisture and soil temperature factors are calculated and the nitrification rate is reduced by the more limiting of these 2 factors.

Denitrification

Denitrification can only occur when the soil moisture contents within the soil exceed the drained upper limit of plant available water and when there is greater than 1 g/Mg of nitrate-nitrogen present. The 2 approaches differ in the calculation of denitrification.

In the 1-D approach a constant denitrification rate is assumed. This rate is then adjusted based on the carbon and nitrate-nitrogen concentrations in the layer and is reduced for limiting soil moisture and soil temperature.

In the 2-D approach, denitrification is based on a dual substrate Michaelis-Mention equation

$$V_{dn} = V_{max} \frac{[C][N]}{([C] + K_C)([N] + K_N)}$$

where [C] is the concentration of carbon, [N] is the concentration of nitrate-nitrogen, K_C and K_N are the Michaelis-Mention constants and V_{max} is the maximum rate of denitrification. The variables V_{max} is equal to 0.15 mg/cm³ and K_C and K_N are assumed to equal 0.17 and 0.50 mg/cm³ water respectively (Bowman and Focht, 1974). The daily amount of nitrogen denitrified is then reduced by either soil moisture or soil temperature factors, whichever is more limiting.

Actual soil evaporation

Soil water is reduced in the surface soil layer to reflect the potential soil evaporative demand of the atmosphere as discussed above. The 2 modeling approaches differ slightly in the reduction of soil moisture in the surface layer. In the 1-D approach the limit to which soil moisture can be reduced in the surface is dependent upon the lower limit of plant available water and the thickness of the surface layer. In the 2-D approach the soil evaporative demand is partitioned first to the unshaded surface area. The amount of potential soil evaporation not met by the unshaded surface area is then partitioned to the shaded surface area.

Soil water in the surface under either approach cannot be reduced below the lower limit of plant available water.

Soil water runoff

Soil water runoff is determined using the SCS curve number method assuming an antecedent moisture content of II and an initial abstraction (I_a) of 2S (SCS, 1972, 1986). The two modeling approaches differ in the calculation of runoff. The 1-D approach uses an average curve number for the entire simulation. The 2-D approach uses a fallow curve number until greater than 1/3 of the maximum leaf area index (LAI) is reached, an average curve number is used when the LAI is between 1/3 and 2/3 of the maximum LAI, and a peak curve number is used when the LAI is greater than 2/3 of the maximum LAI. The peak curve number is calculated as:

$$CN_p = 2 \times CN_a - CN_f$$

where CN_p is the peak curve number, CN_a is the average curve number, and CN_r is the fallow curve number. CN_a and CN_r are input by the user.

Soil water recharge

At the beginning of each day, additions of soil water due to a rainfall or irrigation event are distributed to successive layers in the soil system by bringing each layer to the drained upper limit of plant available water. There is no difference between the modeling approaches with regard to soil water recharge.

Root water uptake

Water is taken up by the roots to meet the potential transpirational demand of the atmosphere as discussed above. The transpirational demand is partitioned to the soil areas containing roots. The transpirational demand partitioned to each area depends on the uptake factor in proportion to the total root zone uptake factor. The 2 modeling approaches differ in the calculation of the uptake factors. Both approaches calculate the uptake factor based on the root weight and soil water diffusivity. However, the method of calculation of the soil water diffusivity differs under the 2 approaches.

In the 1-D approach soil water diffusivity is based on the equation presented by Gardner and Mayhugh (1958).

$$D(\theta) = \alpha e^{\beta\theta}$$

where α and β are constants equal to 0.88 and 35.4 for all simulations and θ is the soil moisture content of the layer.

In the 2-D approach the soil water diffusivity is calculated from the equation presented by van Genuchten (1980)

$$D(\theta) = K \frac{(\theta)}{c}(\theta) = \frac{K_s \Theta^{0.5} [1.0 - (1.0 - \Theta^{1/m})^m]^2}{\alpha(n-1)(\theta_s - \theta_r) \times \Theta^{1/m} (1.0 - \Theta^{1/m})^m}$$

where K is the hydraulic conductivity of a cell and c is the soil moisture capacity of the cell, K_s is the saturated hydraulic conductivity, Θ is the relative soil moisture content, θ_s is the saturated soil moisture content, θ_r is the residual soil moisture content and α , and n are input parameters and m is calculated as

$$m = 1 - \frac{1}{n}$$

Under both approaches the uptake factors for each soil area are summed and the transpirational demand is partitioned to each area based on the area's uptake factor in relation to the total root zone uptake factor. The moisture content of the area is then reduced to reflect plant water uptake. Soil water uptake cannot reduce soil moisture below the lower limit of plant available water in any layer or cell. Should this happen water uptake is reduced and soil moisture response factors are calculated to reduce plant growth.

Root nitrogen uptake

The 2 modeling approaches differ significantly in their calculation of nitrogen uptake by plant roots.

In the 1-D approach the plant uptakes both nitrate and ammonium forms of nitrogen. The amount of each taken up is based on availability factors of nitrate-nitrogen and ammonium-nitrogen and the root weight volume in Kg/ha. A minimum of 1 g/Mg of nitrate-nitrogen and ammonium-nitrogen must be maintained in each soil layer containing roots.

In the 1-D approach nitrogen is taken up to meet the plant nitrogen demand. During growth stage 1 through 4, plant nitrogen demand is determined based on a critical and the actual nitrogen concentrations in the stover and roots of the plant. During growth stage 5, plant nitrogen demand is based on the nitrogen demand of the grain. The nitrogen demand of the grain is determined assuming that the maximum grain protein content is 10 percent.

When the amount of nitrogen taken up by the plant exceeds the plant demand, the uptake is reduced proportionately and only the amount required by the plant is taken up. When the amount of nitrogen taken up by the plant does not meet the plant nitrogen demand nitrogen response factors are calculated to reduce the growth of the plant on the following day.

In the 2-D approach, only nitrate-nitrogen is taken up by the plant roots. Two mechanisms are used to uptake nitrate-nitrogen. Passive nitrate-nitrogen uptake is the uptake of nitrate-nitrogen as mass flow in the soil water taken up by the plant. Active nitrate-nitrogen uptake is described by a Michaelis-Menton first order reaction equation.

Passive nitrate-nitrogen uptake is determined for each cell containing roots as a fraction of the nitrate-nitrogen concentration in the cell to the amount of water taken up from the cell.

Active nitrate-nitrogen uptake is based on the Michaelis-Menton equation presented by Barber (1984) as:

$$V = V_{\max} \left[\frac{[\text{NO}_3] - [\text{NO}_3]_{\min}}{K_m + [\text{NO}_3] - [\text{NO}_3]_{\min}} \right]$$

where V is the net ion influx of nitrate-nitrogen ($\mu\text{moles}/(\text{cm root d})$), V_{\max} is the maximum ion influx of nitrate-nitrogen ($\mu\text{moles}/(\text{cm root d})$), $[\text{NO}_3]$ is the nitrate-nitrogen concentration in the cell ($\mu\text{moles}/\text{ml}$), $[\text{NO}_3]_{\min}$ is the minimum nitrate-nitrogen concentration in the cell below which

plant roots cannot uptake nitrate-nitrogen, and K_m is the Michaelis-Menton constant for root nitrogen uptake.

The work of Edwards and Barber (1976) reported that, for corn roots, the variables K_m and $[\text{NO}_3]_{\min}$ did not vary with the age of the plant. However they did report that V_{\max} decreases exponentially with plant age. From the results presented by Edwards and Barber (1976) a K_m value of 0.01 $\mu\text{moles/ml}$ and a $[\text{NO}_3]_{\min}$ value of 0.004 $\mu\text{moles/ml}$ is assumed. The value of V_{\max} is assumed to vary with plant age according to the equation:

$$V_{\max} = \text{EXP}(-0.7392 - 0.0869P_a)$$

where P_a is the time since plant emergence. This equation was developed from the data of Edwards and Barber (1976) by regressing plant age against the natural log of V_{\max} and obtaining the regression equation:

$$\ln(V_{\max}) = -0.7392 - 0.0869P_a$$

The R^2 value of this equation is 0.9699.

The actual rate of nitrate-nitrogen uptake is then multiplied by the total root length in the cell and both passive and active uptake from all cells are summed and converted to a per plant basis. No limits are placed upon the amount of nitrate-nitrogen which can be taken up during any time step following the 2-D approach.

Soil moisture and nitrate-nitrogen redistribution

After root uptake of water and nitrogen have been accounted for soil moisture and nitrate-nitrogen are redistributed within the soil subsystem. The two modeling approaches differ significantly in their calculation of soil moisture redistribution.

In the 1-D approach, the soil is assumed to be homogeneous and unsaturated soil water redistribution is based on the diffusivity form of Darcy's Law

$$q = \bar{D}(\theta) \frac{\partial \theta}{\partial x}$$

where q is the flux of water between the centers of 2 adjoining layers, and $\bar{D}(\theta)$ is the average soil moisture diffusivity of the adjoining layers. The average soil moisture diffusivity is calculated as

$$\bar{D}(\theta) = \alpha \exp \left[\beta \frac{\theta_{i+1} + \theta_i}{2} \right]$$

where $\alpha = 0.88$, and $\beta = 35.4$ for all simulations and θ_{i+1} and θ_i are the soil moisture contents of the 2 adjoining layers. Positive values for q indicate upward movement of water and negative values indicate downward movement of water.

The net change in soil moisture content in a layer is determined as the net gain or loss of water between the centers of the adjoining layers calculated as

$$\frac{\partial \theta}{\partial t} = \frac{\partial q}{\partial x}$$

In the 2-D approach, the soil is inhomogeneous and unsaturated soil moisture redistribution is based on the equation:

$$q_y = \bar{K}(\theta)_y \frac{\partial h}{\partial y}$$

$$q_x = \bar{K}(\theta)_x \frac{\partial H}{\partial x}$$

where h is pressure head (cm) and H is hydraulic head (cm). $\bar{K}(\theta)_y$ is the harmonic mean hydraulic conductivity of 2 adjoining cells in the horizontal direction and $\bar{K}(\theta)_x$ is the harmonic mean hydraulic conductivity of 2 adjoining cells in the vertical direction. The harmonic means are calculated as

$$\bar{K}(\theta)_x = \frac{2}{\frac{1}{K(\theta)_x} + \frac{1}{K(\theta)_{x+1}}}$$

$$\bar{K}(\theta)_y = \frac{2}{\frac{1}{K(\theta)_y} + \frac{1}{K(\theta)_{y+1}}}$$

The hydraulic conductivity of each cell is calculated from the equation presented by van Genuchten (1980):

$$K(\theta) = K_s \Theta^{1/2} [1.0 - (1.0 - \Theta^{1/m})^m]^2$$

where K_s is the saturated hydraulic conductivity, m is a constant parameter, and Θ is the relative soil moisture content of the cell defined by van Genuchten (1980) as:

$$\Theta = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1.0}{1.0 + (\alpha h)^n} \right]^m$$

where θ is the current soil moisture content of a cell, θ_r is the residual soil moisture content, θ_s is the saturated soil moisture content, and α , and n are input parameters, and $m = 1 - 1/n$.

The variables θ_r , θ_s , α , n , and K_s are input by the user. The variable h is calculated as:

$$h = \frac{1}{\alpha} (\Theta^{1/m} - 1.0)^{1/n}$$

Positive values for q indicate gain in moisture in a cell and negative values indicate loss of water from a cell. The net change in soil moisture content in a cell is determined as the net gain or loss of water to all adjacent cells in the vertical and horizontal directions calculated as

$$\frac{\partial \theta}{\partial t} = \frac{\partial q_y}{\partial y} + \frac{\partial q_x}{\partial x}$$

At the bottom boundary the user may specify either a unit gradient or a water table.

In both the 1-D and 2-D approaches, nitrate-nitrogen in the soil is redistributed by mass flow. The redistribution of nitrate-nitrogen is calculated as

$$q_n = q_w \times \frac{[\text{NO}_3]}{\theta}$$

where q_n is the flux density of nitrate-nitrogen, q_w is the flux density of water, $[\text{NO}_3]$ is the nitrate-nitrogen concentration, and θ is the soil moisture content. In the 1-D approach the net increase or decrease in nitrate-nitrogen in a layer is then calculated as

$$\frac{\partial[\text{NO}_3]}{\partial t} = \frac{\partial q_n}{\partial x}$$

and in the 2-D approach as

$$\frac{\partial[\text{NO}_3]}{\partial t} = \frac{\partial q_{ny}}{\partial y} + \frac{\partial q_{nx}}{\partial x}$$

Response Mechanisms

The response mechanisms described below refer to the effects produced on the plant by the atmosphere and soil subsystems. These responses include an atmospheric temperature factor, two soil water deficit factors, and two nitrogen deficit factors.

Atmospheric temperature response

The atmospheric temperature factor assumes optimum production of carbohydrates by the corn plant at 26°C and reduces carbohydrate production proportionately when the average daily temperature, adjusted for day length, is greater or less than this optimum.

Soil water deficit response

The two soil water deficit factors are determined daily to represent the lack of soil moisture supplied to the plant to meet the transpirational demand of the atmosphere. The first soil water deficit factor reduces carbohydrate production during photosynthesis and transpiration and is calculated as the ratio of the actual transpiration to potential transpiration. The second soil water deficit factor reduces the rate of cell elongation which in turn reduces the rate of increase of the LAI of the crop. The second soil water deficit factor is calculated as 67 percent of the first soil water deficit factor when the first soil water deficit factor is less than 1.0. Neither soil water deficit factor is allowed to exceed a value of 1.0.

Nitrogen deficit response

Two separate approaches to the calculation of nitrogen deficit factors are used depending on whether the 1-D or 2-D approach is used. The first nitrogen deficit factor affects the daily production of carbohydrates, the second affects leaf senescence. Under both modeling approaches there are 2 methods of determining the nitrogen deficit factors which are dependent upon the growth stage of the plant.

In the 1-D approach the nitrogen deficit factors are calculated as the ratio of the amount of nitrogen taken up by the plant to the nitrogen demand of the plant. The plant nitrogen is growth stage dependent. During growth stages 1 through 4, the plant nitrogen demand is calculated based on the critical and actual nitrogen concentrations of the stover and roots. During growth stage 5 the plant nitrogen demand is calculated based on the daily grain nitrogen demand.

The difference between the 2 nitrogen deficit factors is that the first nitrogen deficit factor is equal to 1.0 unless the ratio of nitrogen taken up to plant nitrogen demand is less than 0.80. When the ratio is less than 0.8 the first nitrogen deficit factor is 1.25 times the ratio. The second nitrogen deficit factor is equal to the ratio of nitrogen uptake to plant nitrogen demand.

In the 2-D approach nitrogen deficit factors are based on the root shoot relationship and the identity presented by Charles-Edwards (1982):

$$W_T \frac{\sigma_T}{f_C} = W_R \frac{\sigma_R}{f_M} \quad [1]$$

where W_T is the shoot weight of the plant, W_R is the root weight of the plant, σ_T is the specific activity of the shoots to produce carbon, σ_R is the specific activity of the roots to uptake a specific nutrient species and f_C and f_M are the elemental carbon and nutrient concentrations in the plant, respectively, and are defined as:

$$f_C = \frac{\Delta C}{\Delta W}$$

$$f_M = \frac{\Delta M}{\Delta W}$$

where $\Delta C/\Delta W$ is the unit increase in carbon content of the plant required per unit change in weight of the plant and $\Delta M/\Delta W$ is the unit increase in a nutrient required per unit change in weight of the plant.

Assuming that the nutrient of interest is nitrogen and rearranging equation 1 the following identity is defined.

$$E_\sigma = \frac{\sigma_R}{\sigma_T} = \frac{f_{N_s} W_T}{f_C W_R}$$

where E_σ is the expected ratio of the specific activity of the tops to produce carbon to the specific activity of the roots to uptake the nutrient nitrogen. If we assume that $f_C = 0.40$, is the fractional carbon content of a unit of structural carbohydrate and that f_{N_s} is the optimum fractional nitrogen content of a corn plant, then the expected specific activity E_σ can be defined as:

$$E_\sigma = \frac{f_{N_s} W_T}{0.40 W_R}$$

The same approach can be taken in the determination of the actual ratio of the specific activities (A_σ):

$$A_\sigma = \frac{f_{N_s} W_T}{f_C W_R}$$

where f_C is again assumed to equal 0.40, however f_{N_s} is defined as:

$$f_{N_s} = \frac{\Delta N}{\Delta W}$$

where ΔN is the amount of nitrogen taken up over the time step and ΔW is the potential total plant carbohydrate produced over the same time step.

From these definitions a nitrogen deficit factor can be determined as the ratio of actual to expected activities:

$$N_{def} = \frac{A_{\sigma}}{E_{\sigma}} = \left[\frac{f_{Na} W_T}{f_C W_R} \right] \times \left[\frac{f_C W_R}{f_{Ne} W_T} \right]$$

Reduction of this equation gives

$$N_{def} = \frac{f_{Na}}{f_{Ne}}$$

and by substitution:

$$N_{def} = \frac{\Delta N_a}{f_{Ne} \Delta W}$$

where ΔN_a is the amount of nitrogen taken up by the plant over a time step and ΔW is the potential weight change of the plant over the same time step and the value of f_{Ne} is determined based on the growth stage of the plant as

$$f_{Ne} = 0.04 \qquad \text{ISTAGE} \leq 4$$

$$f_{Ne} = 0.10/6.25 \qquad \text{ISTAGE} = 5$$

where it is assumed that the optimum nitrogen content of the vegetative portion of the plant is 4 percent of the plant weight. During growth stage 5, or grain fill, it is assumed that the carbohydrate produced is to be partitioned to the grain and that the maximum grain protein content is 10 percent and 6.25 is the conversion factor for converting protein to nitrogen.

Two nitrogen deficit factors are then calculated. The first nitrogen deficit factor, which affects photosynthesis, is equal to 1.0 unless the value of N_{def} is less than 0.80. When N_{def} is less than 0.8 the first nitrogen deficit factor is 1.25 times the value of N_{def} . The second nitrogen deficit factor is equal to the value of N_{def} .

The above approach has been used in the interest of later incorporation of other nutrient affects on plant growth. Charles-Edwards (1982) shows that the individual identities:

$$\frac{f_M}{\sigma_R} = \frac{W_R}{\Delta W / \Delta t}$$

$$\frac{f_C}{\sigma_T} = \frac{W_T}{\Delta W / \Delta t}$$

are additive, and the total dry weight of the plant can be explained as:

$$\frac{f_M}{\sigma_R} + \frac{f_C}{\sigma_T} = \frac{(W_R + W_T)}{\Delta W / \Delta t}$$

and further, that the same additive property applies to multiple nutrients such that:

$$\sum_{n=1}^m \left(\frac{f_M}{\sigma_R} \right)_n + \frac{f_C}{\sigma_T} = \frac{(nW_R + W_T)}{\Delta W / \Delta t}$$

From this, the same additive property applies to equation 1 such that:

$$W_T \frac{\sigma_T}{f_C} = nW_R \sum_{n=1}^m \left(\frac{\sigma_R}{f_M} \right)_n$$

We can go through a proof similar to the above to show that:

$$M_{def} = \frac{A_\sigma}{E_\sigma} = \frac{\sum_{n=1}^m (f_{Ma})_n}{\sum_{n=1}^m (f_{Ma})_n \times \Delta W}$$

where M_{Def} is an overall nutrient deficit factor affecting plant growth.

The above equation will allow not only for incorporation of multiple nutrient effects on the plant using one response factor but also will allow for the incorporation of nutrient interactions when these interactions are incorporated into root uptake processes.

Chapter 2: Preliminary Evaluation of the Simulation

Model C-Maize VT1.0

Introduction

The initial simulation runs of the C-Maize VT1.0 program were designed to evaluate the performance of each of the 2 approaches within the C-Maize model. The runs included a standard run, a series of runs to evaluate the sensitivity of the model, and a calibration test. A preliminary credibility assessment of the C-Maize VT1.0 model was also performed by the persons directly involved in the development of the model.

Materials and Methods

The following describes the initial runs made to evaluate the C-Maize VT1.0 simulation model. Tables 3 and 4 describe the crop, soil, and site characteristics used for all simulations under both the 1-D and 2-D approaches, respectively, with exceptions as noted below. The soil moisture conditions under the 1-D approach differs from the moisture conditions under the 2-D approach. Soil moisture conditions for the 2-D approach were generated from the characterization data presented by Kool et al. (1986) for a Groseclose Silt Loam mapping unit. The 1-D approach could not be made to run under the same soil moisture range as the 2-D approach and was therefore calibrated to a soil moisture range within which the model would run. Although the models cannot be directly compared general statements about the performance of each approach can be made.

Standard Simulation

The purpose of the standard runs was to evaluate the performance of the test system under both the 1-D and 2-D approaches. These runs also represent the control system for the sensitivity

Table 3. Input parameters used for running 1-D simulations

Program begins simulation on day - 121

Plant Characteristics:

Cultivar - Dekalb XL71
 Plant population - 6.0 pl/m²
 Sowing date - 131

Genetic Constants:

P1 - 140.00 (°C) G2 - 825.40 (kernels/plant)
 P2 - 0.30 (1/hr) G3 - 10.50 (mg/kernal d)
 P3 - 685.00 (°C)

Soil Characteristics:

Albedo - 0.14 Swcon - 4.97
 U - 9.00mm Average Curve Number - 85.00

Depth	θ_{11}	θ_{dul}	θ_{sat}
(cm)	----- cm/cm -----		

0 - 15	0.10	0.45	0.46
15 - 25	0.10	0.45	0.46
25 - 55	0.11	0.48	0.49
55 - 75	0.11	0.48	0.49
75 -105	0.26	0.56	0.58
105 -135	0.26	0.56	0.58
135 -165	0.26	0.56	0.58
165 -195	0.26	0.56	0.58
195 -225	0.26	0.56	0.58

Table 4. Input parameters used for running 2-D simulations

Program begins simulation on day - 121

Plant Characteristics:

Cultivar - Dekalb XL71
 Plant population - 6.0 pl/m²
 Sowing date - 131

Genetic Constants:

P1 - 140.00 (°C) G2 - 825.40 (kernels/plant)
 P2 - 0.30 (1/hr) G3 - 10.50 (mg/kernal d)
 P3 - 685.00 (°C)

Soil Characteristics:

Albedo - 0.14 Average Curve Number - 85.00
 U - 9.00mm Fallow Curve Number - 91.00

Cell dimensions - 5.0 X 5.0 cm 40 X 10

Depth	θ_r	θ_{15}	θ_{dul}	θ_{sat}	K_s	alpha	n
(cm)	----- cm ³ /cm ³ -----			-----	cm/d	1/cm	

0 - 30	0.160	0.210	0.331	0.410	126.000	0.10	1.22
30 - 80	0.280	0.284	0.350	0.420	252.000	0.07	1.51
80 -200	0.430	0.436	0.510	0.530	0.159	0.02	1.48

analyses and the test calibration runs. Initial soil moisture conditions for these runs were assumed to be field capacity. Each run also included the addition of 250 kg/ha of ammonium fertilizer on the day the crop was planted. The purpose of the standard runs was to evaluate the performance of each model for a number of critical variables. These variables included growth of individual plant parts and changes in soil temperature, organic matter, ammonium-nitrogen, and nitrate-nitrogen in the soil profile with time.

Sensitivity Analysis

Sensitivity analysis involves changing the value of one variable or parameter and evaluating the results of these changes. In the following series of runs one parameter or variable in the standard simulation was changed and the simulated results were evaluated. The first series of runs evaluated the difference in initial moisture contents under both the 1-D and 2-D approaches. Initial moisture contents were assumed to vary as a fraction of field capacity. The second series of runs evaluated the effect of rainfall under both the 1-D and 2-D approaches. Rainfall was varied as a fraction of daily rainfall received. This method allowed the remaining climatic variables to remain constant. The initial moisture condition for all runs was assumed to be at field capacity. The third series of runs evaluated the effect of applied nitrogen fertilizer on grain yield. Three types of fertilizer, ammonium, ammonium-nitrate, and nitrate, were applied at rates of 0, 50, 100, 150, 200, and 250 kg/ha.

Calibration

Actual field experiments have not yet been performed to either calibrate or evaluate the C-Maize VT1.0 model. However, a test case was performed to determine whether or not the model could be calibrated to an individual management system. For this test 3 varieties of corn from the 1985 Virginia Corn Performance Trials held at Blacksburg, Virginia (Donahue et al., 1985) were selected for calibration. These trials were selected because they were held in an area with a soil type of Groseclose Silt Loam and the weather data for 1985 could be used. The soil and weather data are the same data used in the standard runs. The tests were run assuming an initial moisture content of field capacity. Two applications of 110 kg/ha of ammonium fertilizer were applied at planting and at the end of growth stage 2. Plant populations for each variety reflected the final plant populations of the field experiments. For this test the crop genetic parameters (Molten et al., 1987a) were varied until simulated results closely approximated the final field results. Only 2 variables could be evaluated during the test calibration, silking date and final grain yield.

Preliminary Credibility Assessment

The process of credibility assessment in simulation modeling assures that a simulation model is evaluated for completeness and accuracy during all phases of development and allows for the quantitative assessment of the model and the model results. Balci (1986a) describes the life cycle of a simulation modeling project (Figure 5). Balci (1986b) describes three types of error which may occur during a simulation project. Type I error, or model builder's risk, is committed when the project's results are rejected when they are sufficiently credible. Type II error, or model user's risk, occurs when the project's results are accepted when they are not sufficiently credible. Type III error

is committed when the formulated problem does not contain the actual problem. Figure 6 (Balci, 1986b) outlines the steps used to assure that a simulation model is acceptable, credible, and describes the system being simulated. Following this hierarchy minimizes the probability of committing errors of type I, II, or III.

To quantitatively evaluate a model's credibility a weighting factor (W) is assigned to each branch at each step of each level in the credibility hierarchy (Figure 6). The weighting factors within the hierarchy must satisfy the condition

$$\sum_{k=1}^{n_{ijk}} W_{ijk} = 1.0$$

where W_{ijk} is the weight assigned to the k branch of at step j , at level i of the hierarchy. A panel of judges knowledgeable of the system being simulated, evaluates each k branch by assigning a relative score (0 to 100) to reflect the credibility of each aspect of the hierarchy. The relative scores (S) of each branch are multiplied by the weighting factor of the branch and summed at each step to obtain the score at the next successively higher level in the hierarchy

$$S_{ij} = \sum_{k=1}^n W_{ijk} \times S_k$$

The score at each successively higher level is calculated until an overall score is attained at the credibility assessment step (Figure 6). Scores between 0 and 100 represent relative levels of credibility. A score of 0 represents 'not credible' while a score of 100 represents 'sufficiently credible'.

For the purpose of this study a preliminary assessment (Figure 7) of the C-Maize model was conducted. For this preliminary assessment the model and the results were evaluated by a panel consisting of a soil physicist (SP), agricultural climatologist (AC), plant physiologist (PP) and system analyst (SA). Each judge's individual score was calculated according to the percentages assigned in Figure 7. The overall score for each approach was calculated by assigning weighting factors to each judge's response, with higher weights given to each judge in his area of expertise. All judge's responses were weighted equally except at level 4 steps 1 through 4 and at level 5 steps 1 through 4 of the hierarchy. Table 5 shows the weights assigned to each judge at these levels.

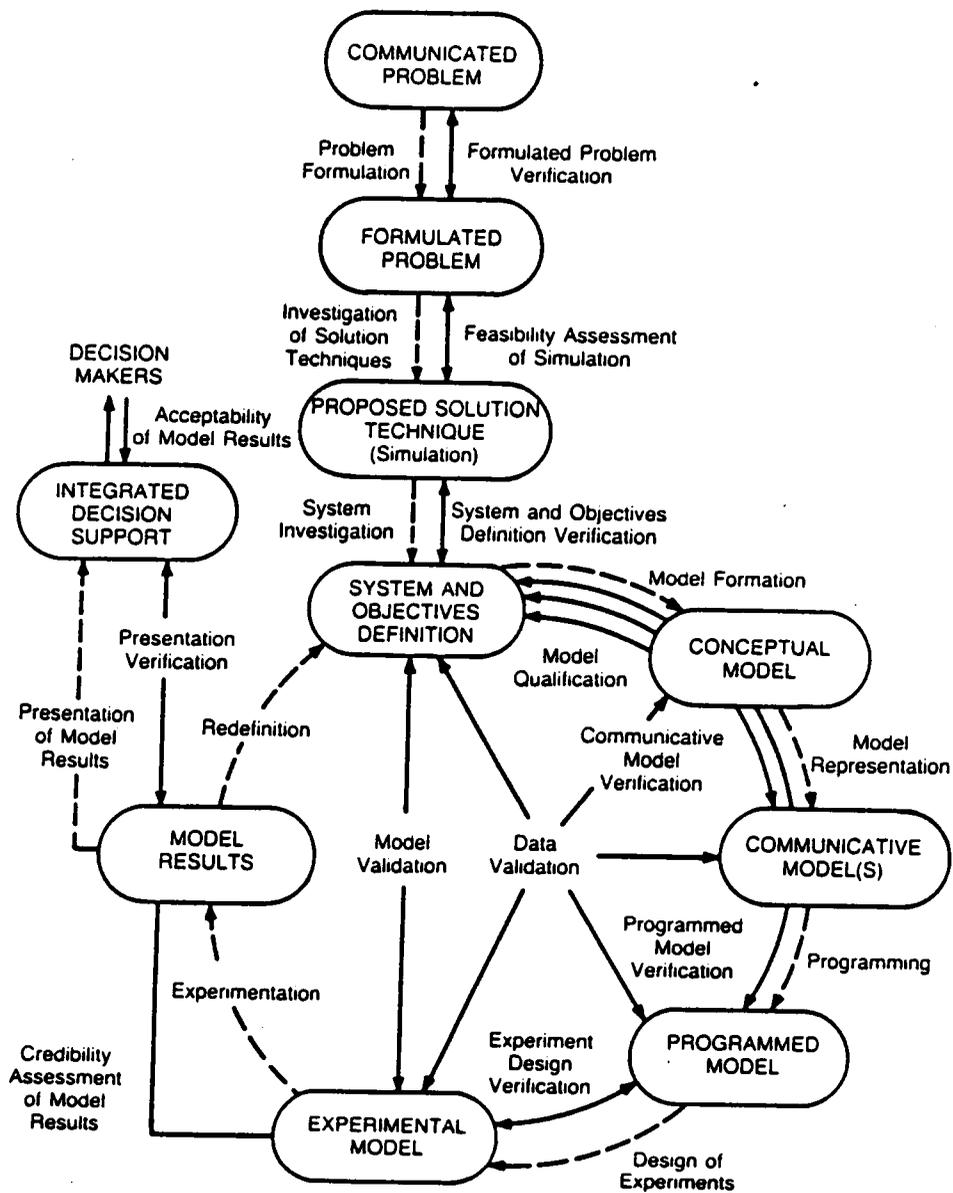


Figure 5. Life Cycle of a Simulation Modeling Project (Balci, 1986)

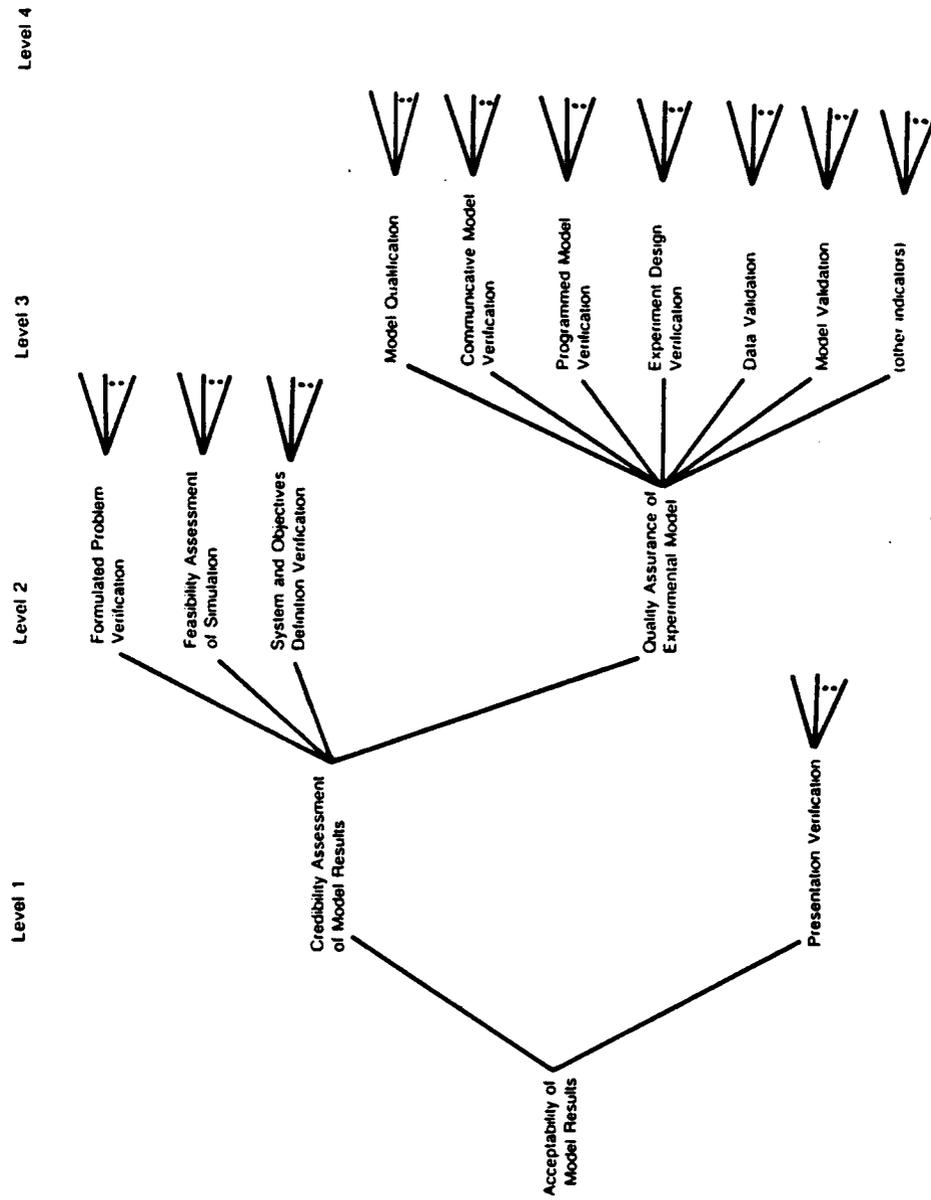


Figure 6. Hierarchy of Credibility Assessment of Simulation Modeling (Balci, 1986)

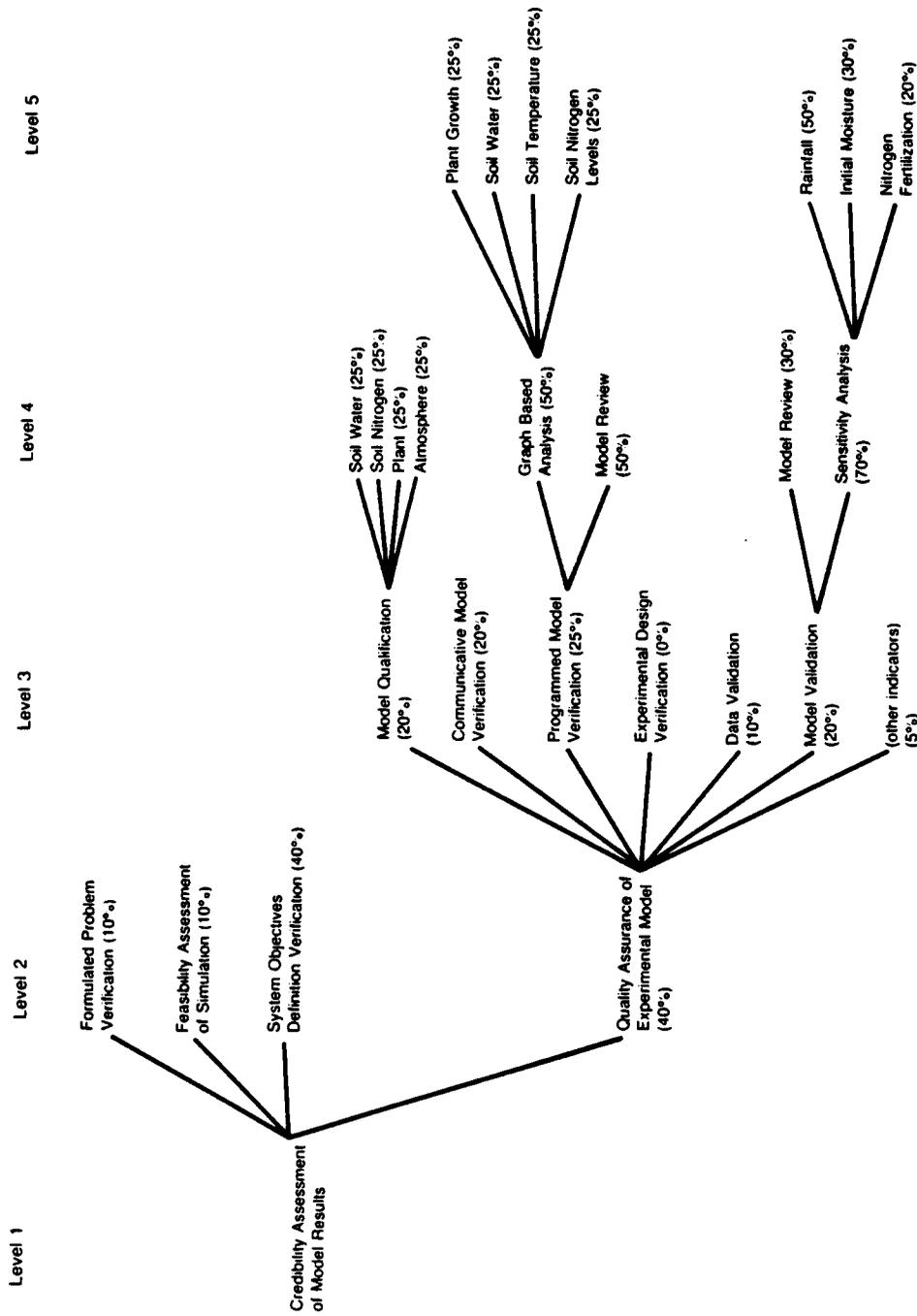


Figure 7. Hierarchy of Preliminary Assessment of C-Maize VT1.0

Table 5. Weighting factors assigned to each judge at levels 4 and 5 of credibility assessment hierarchy

	SP	AC	PP	SA
Level 4:				
Step 1 - Soil water	0.50	0.20	0.10	0.20
Step 2 - Soil nitrogen	0.25	0.25	0.25	0.25
Step 3 - Plant	0.10	0.20	0.50	0.20
Step 4 - Atmosphere	0.10	0.50	0.20	0.20
Level 5:				
Step 1 - Plant growth	0.10	0.20	0.50	0.20
Step 2 - Soil water	0.50	0.10	0.20	0.20
Step 3 - Soil temperature	0.40	0.40	0.10	0.10
Step 4 - Soil nitrogen	0.25	0.25	0.25	0.25

Results and Discussion

Standard Simulation

Figures 8 and 9 show the increase in weight of plant parts through the growing season under the 1-D and 2-D approaches, respectively. Both approaches show approximately the same increase in weight of leaf, stems, and grain. However, root weights under the 2 approaches are significantly different. Figure 10 shows the difference between shoot:root ratios under the 1-D and 2-D approaches compared to the field data collected by Foth (1962). The difference between the 1-D and 2-D approaches is due to the assumptions made about respiratory losses of carbohydrates. The 1-D approach assumes 50 percent loss of root carbohydrate to respiration while the 2-D approach assumes only a 30 percent loss of root carbohydrate to respiration. Both approaches follow the general trend in shoot:root ratios observed by Foth (1962).

Figures 11 and 12 show the soil temperature profiles at different times over the growing season. Both approaches show the expected trend in soil temperature distribution with time and depth.

Figures 13 through 18 show the changes in organic matter, ammonium-nitrogen, and nitrate-nitrogen with depth and time through the growing season. Each approach shows a regular decrease in organic matter content (Figures 13 and 14). The 1-D approach shows a much higher

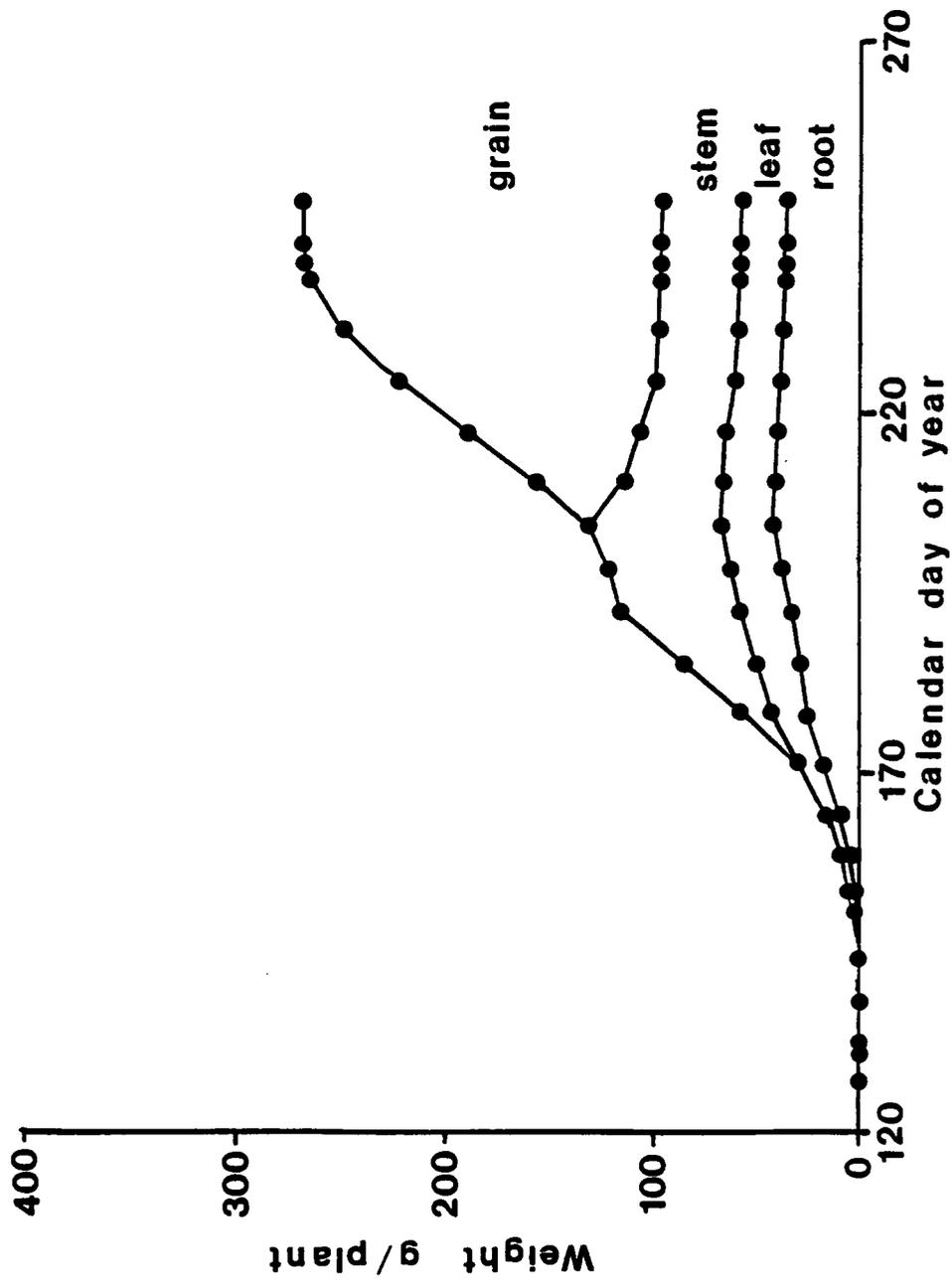


Figure 8. Changes in Weight of Plant Parts with Time Following the 1-D Approach

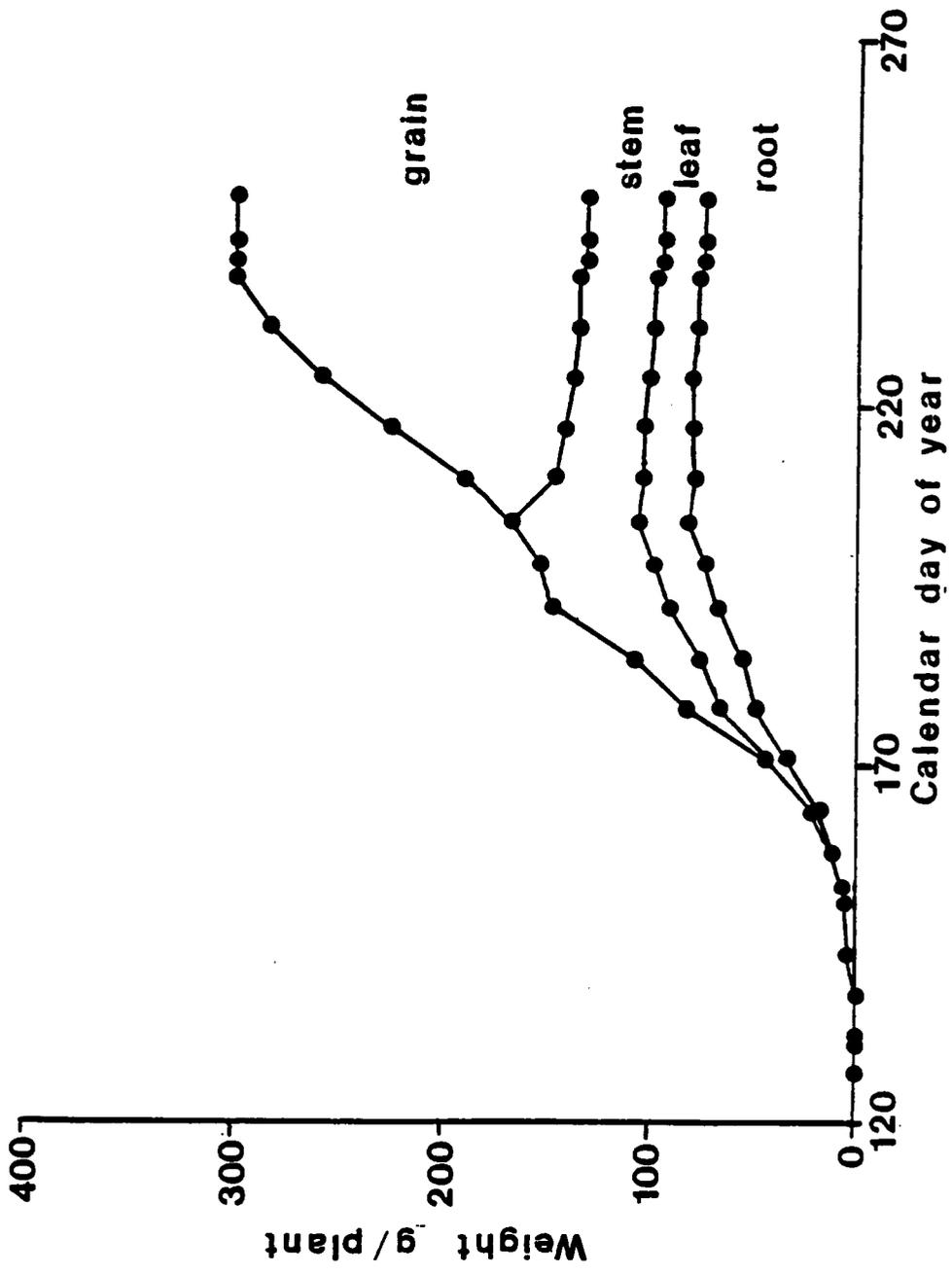


Figure 9. Changes in Weight of Plant Parts with Time Following the 2-D Approach

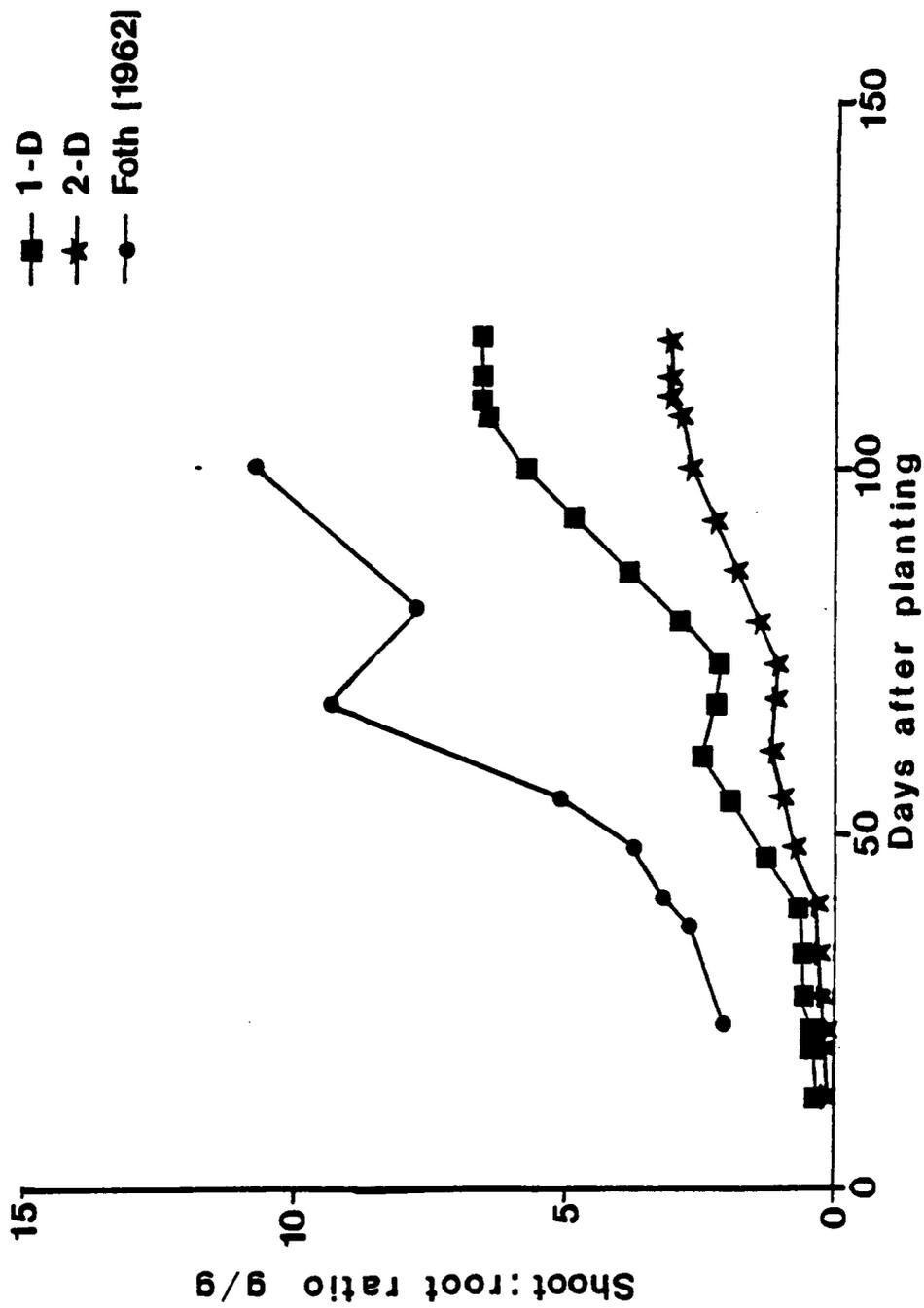


Figure 10. Shoot:root Ratio of 1-D and 2-D Approaches Compared to Observed Shoot:root Ratios of Foth (1962)

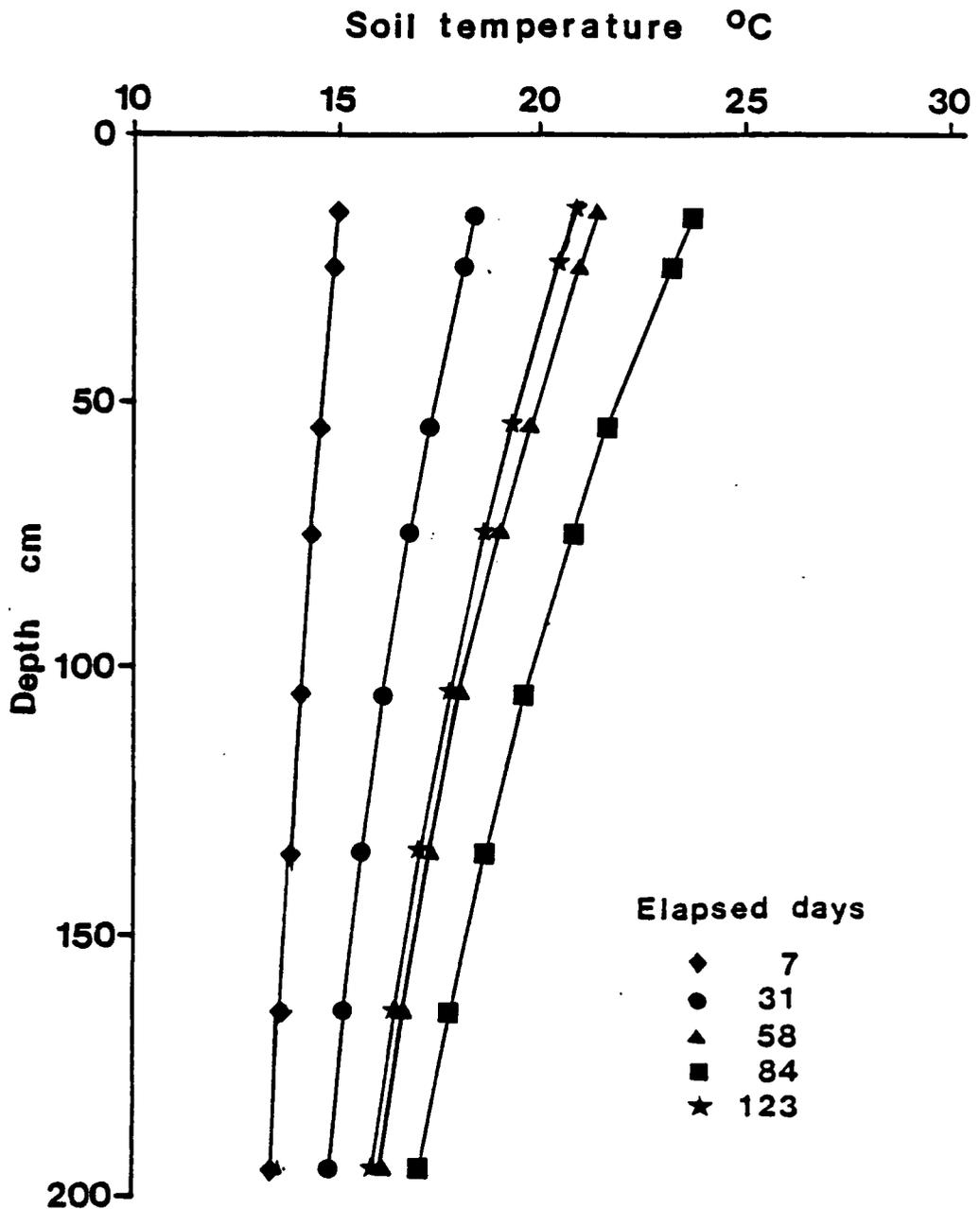


Figure 11. Changes in Soil Temperature Profile with Time Following the 1-D Approach

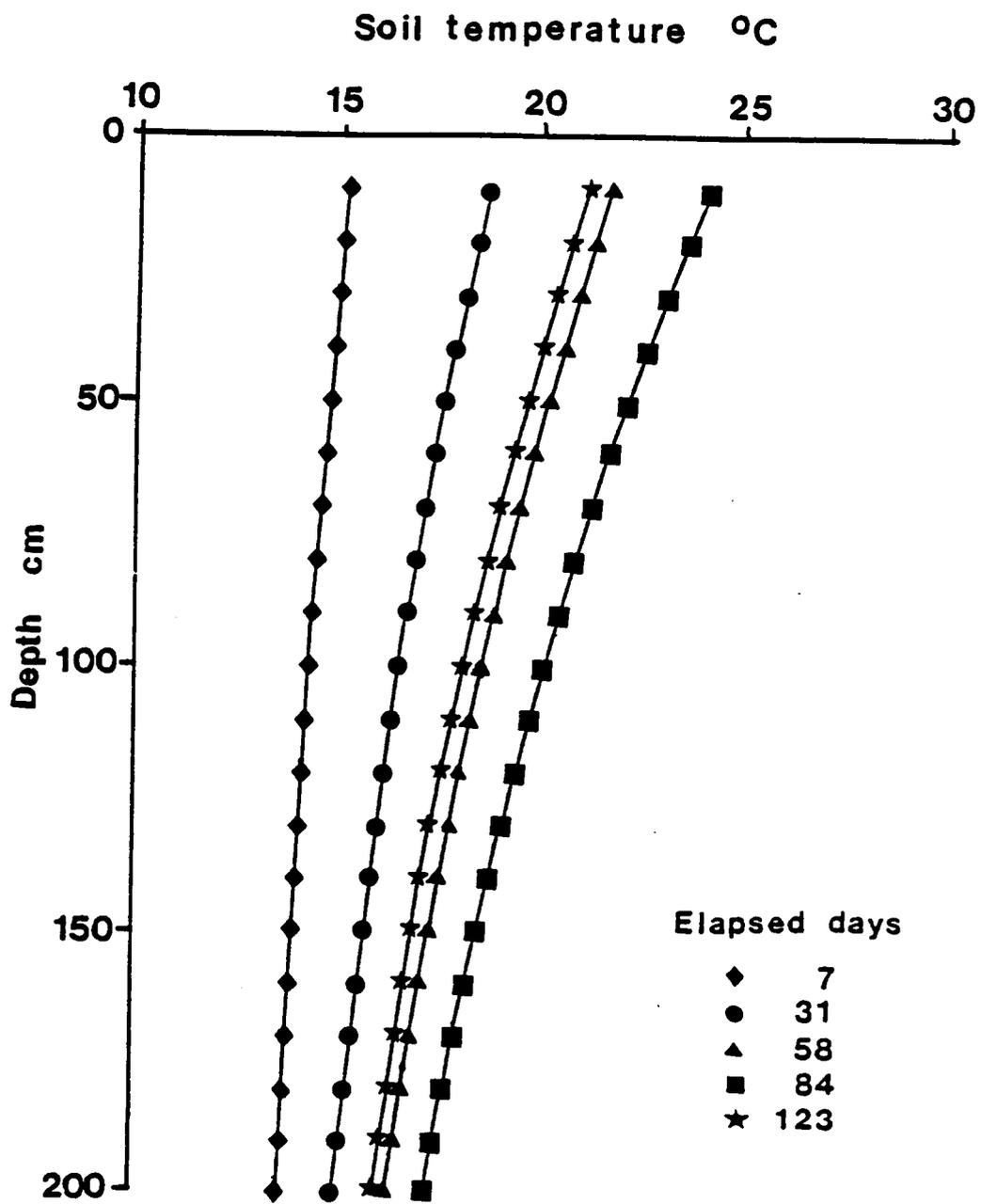


Figure 12. Changes in Soil Temperature Profile with Time Following the 2-D Approach

ammonium-nitrogen content in the profile than does the 2-D approach (Figures 15 and 16). Both approaches show the same general decrease to 84 days and a slight increase at 123 days. The difference in the amounts is due to the nitrification capacity factor, used in the 1-D approach, limiting the rate of nitrification and thus greater concentrations of ammonium-nitrogen remain in the system. Figures 17 and 18 show the distribution of nitrate-nitrogen in the soil profile across the growing season. The 1-D approach shows no movement of nitrate-nitrogen in the profile. The 2-D approach shows movement of a nitrate-nitrogen front in the soil profile.

Sensitivity Analysis

Figures 19 and 20 show, respectively, the effects of varying initial moisture contents and rainfall under both the 1-D and 2-D approaches. The 1-D approach shows a high sensitivity to initial moisture content and a low sensitivity to the amount of rainfall applied. The 2-D approach is much more sensitive to rainfall than it is to initial moisture content. During the 1985 growing season rainfall was 423 mm distributed fairly evenly over the growing season. Evapotranspiration amounted to 416 mm under both approaches. Thus, the amount of rainfall received easily accounted for the evapotranspirational losses. The response of the 2-D approach under this system is more in line with the expected response of the system than is the 1-D approach.

Figures 21 and 22 show the sensitivity of the 1-D and 2-D approaches to the type and amount of nitrogen fertilizer applied. Under the 1-D approach the yield estimates show the effect of allowing for uptake of ammonium-nitrogen and nitrate-nitrogen by the plant. The 1-D approach shows expected response to applications of ammonium and ammonium-nitrate fertilizers. The response to applications of nitrate fertilizers was much lower than expected. The 2-D approach shows little difference between type of nitrogen fertilizer applied. The yield estimates made at application rates of 50 Kg/ha and 100 Kg/ha are somewhat greater than expected. This can be attri-

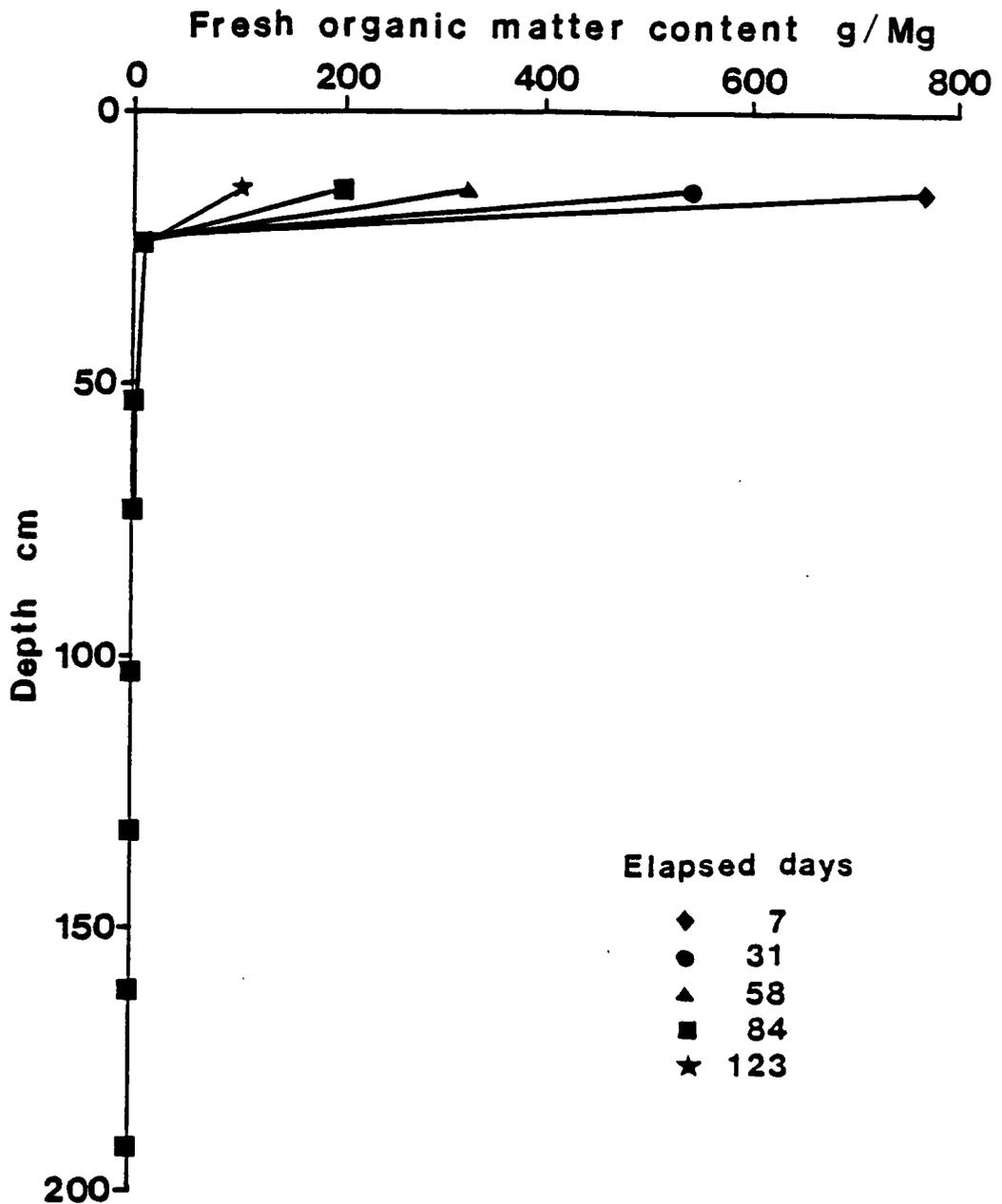


Figure 13. Changes in Organic Matter Profile with Time Following the 1-D Approach

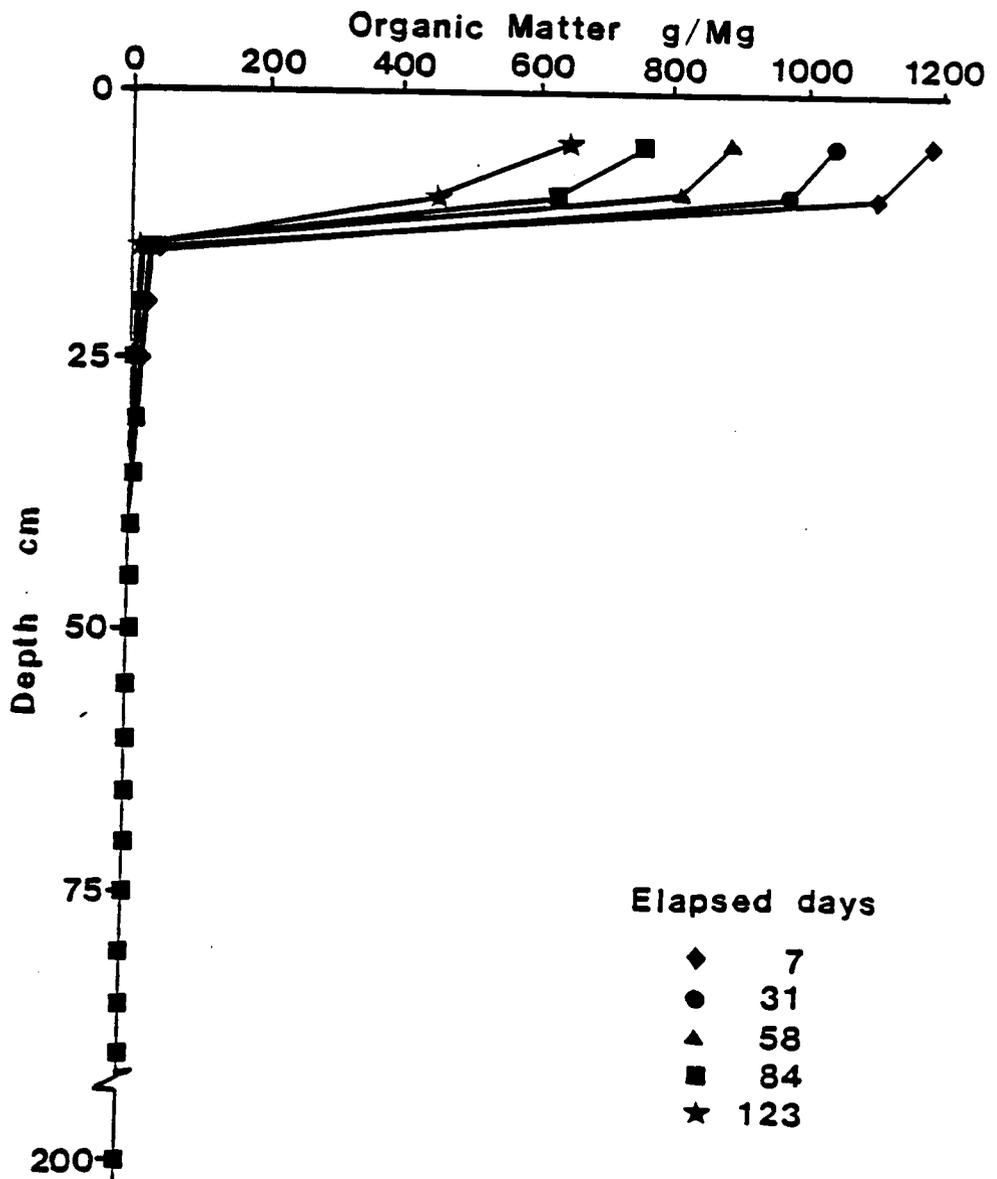


Figure 14. Changes in Organic Matter Profile with Time Following the 2-D Approach

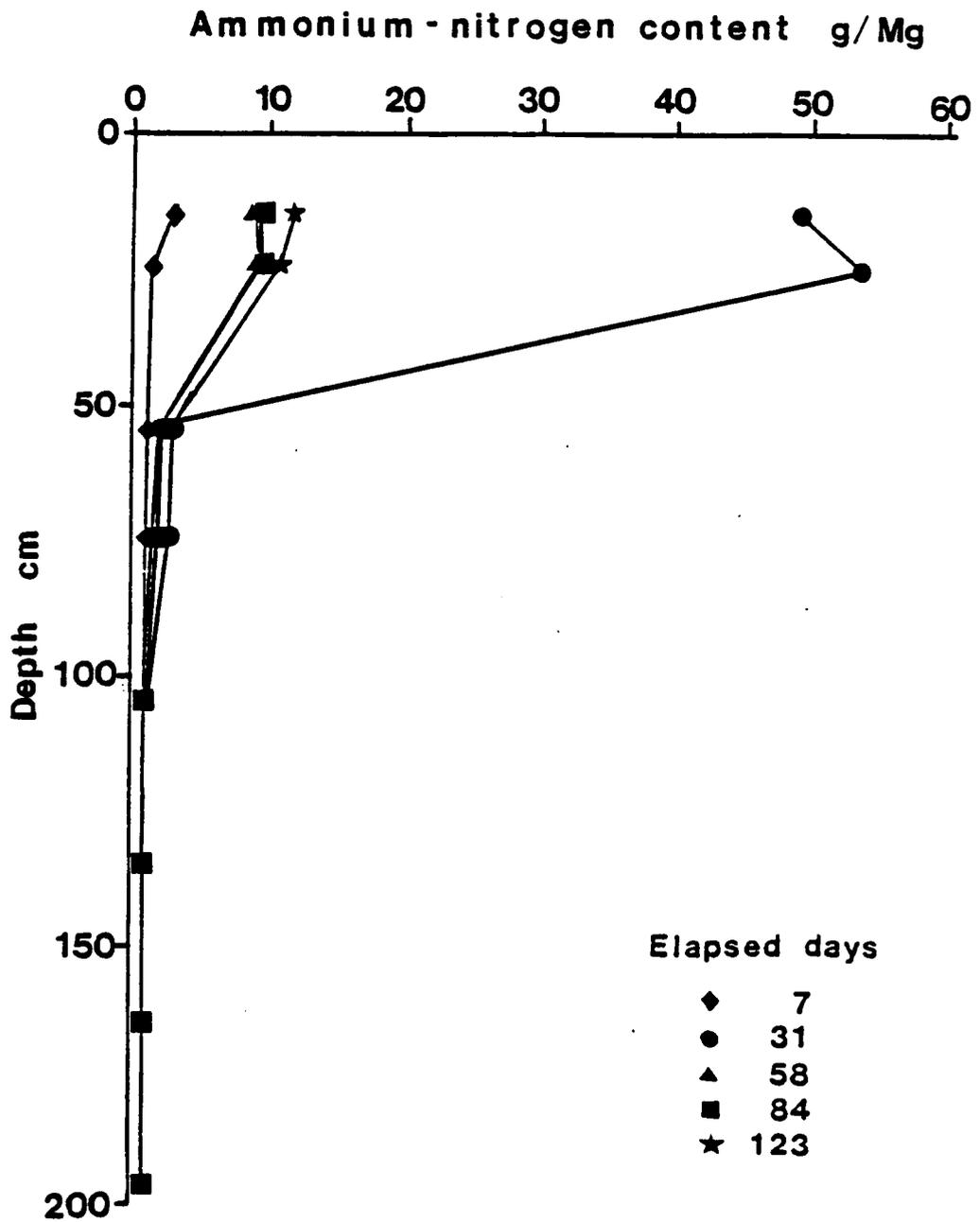


Figure 15. Changes in Ammonium-Nitrogen Profile with Time Following the 1-D Approach

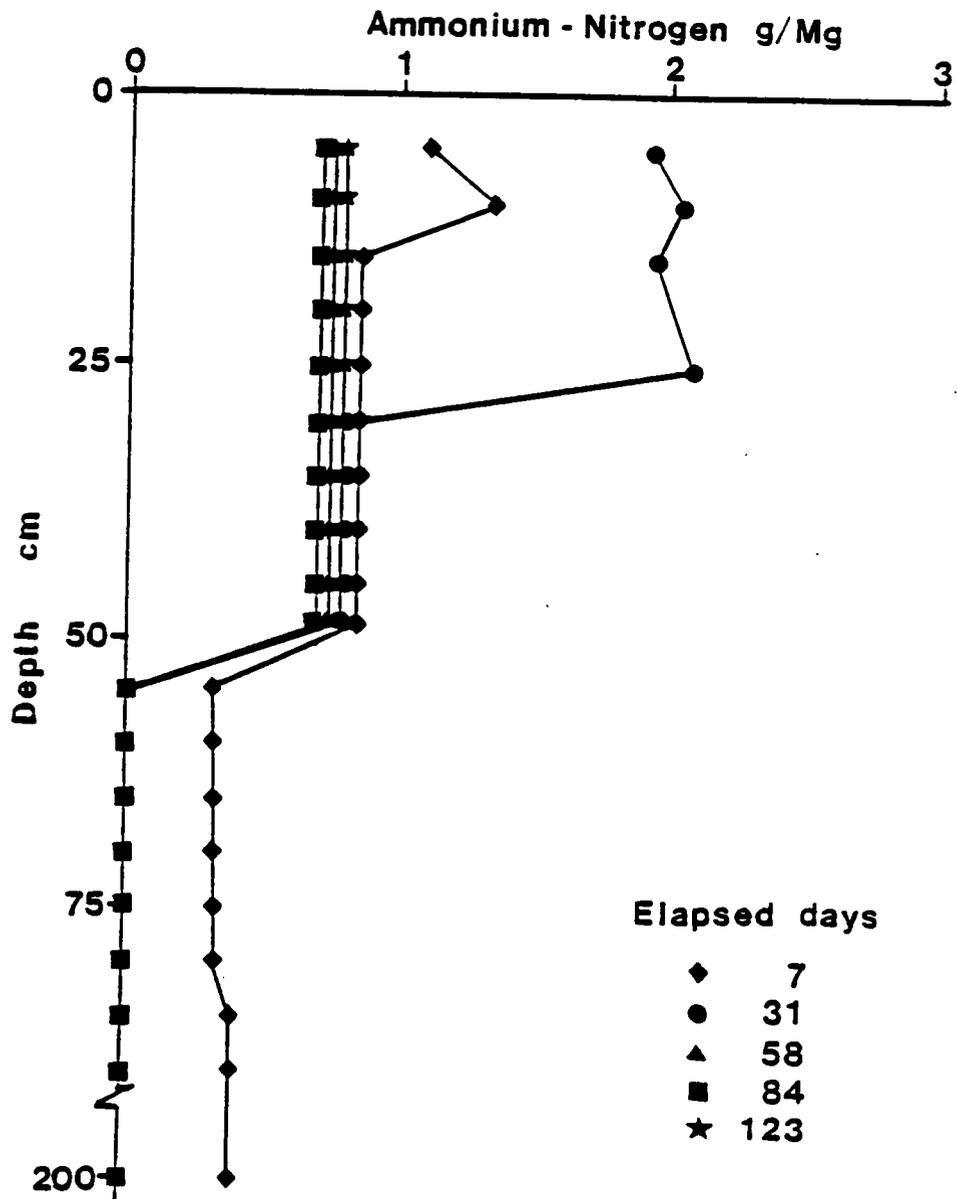


Figure 16. Changes in Ammonium-Nitrogen Profile with Time Following the 2-D Approach

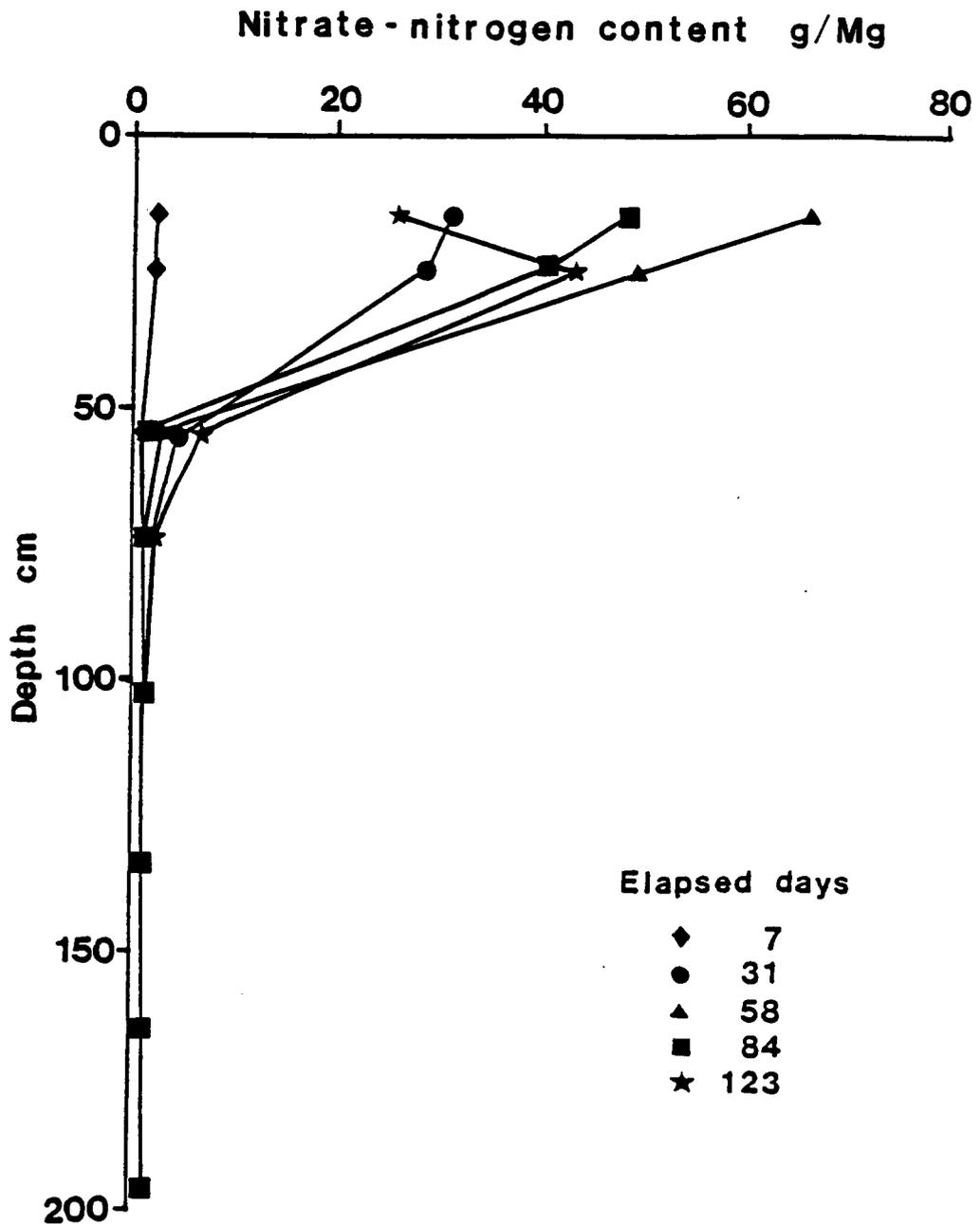


Figure 17. Changes in Nitrate-Nitrogen Profile with Time Following the 1-D Approach

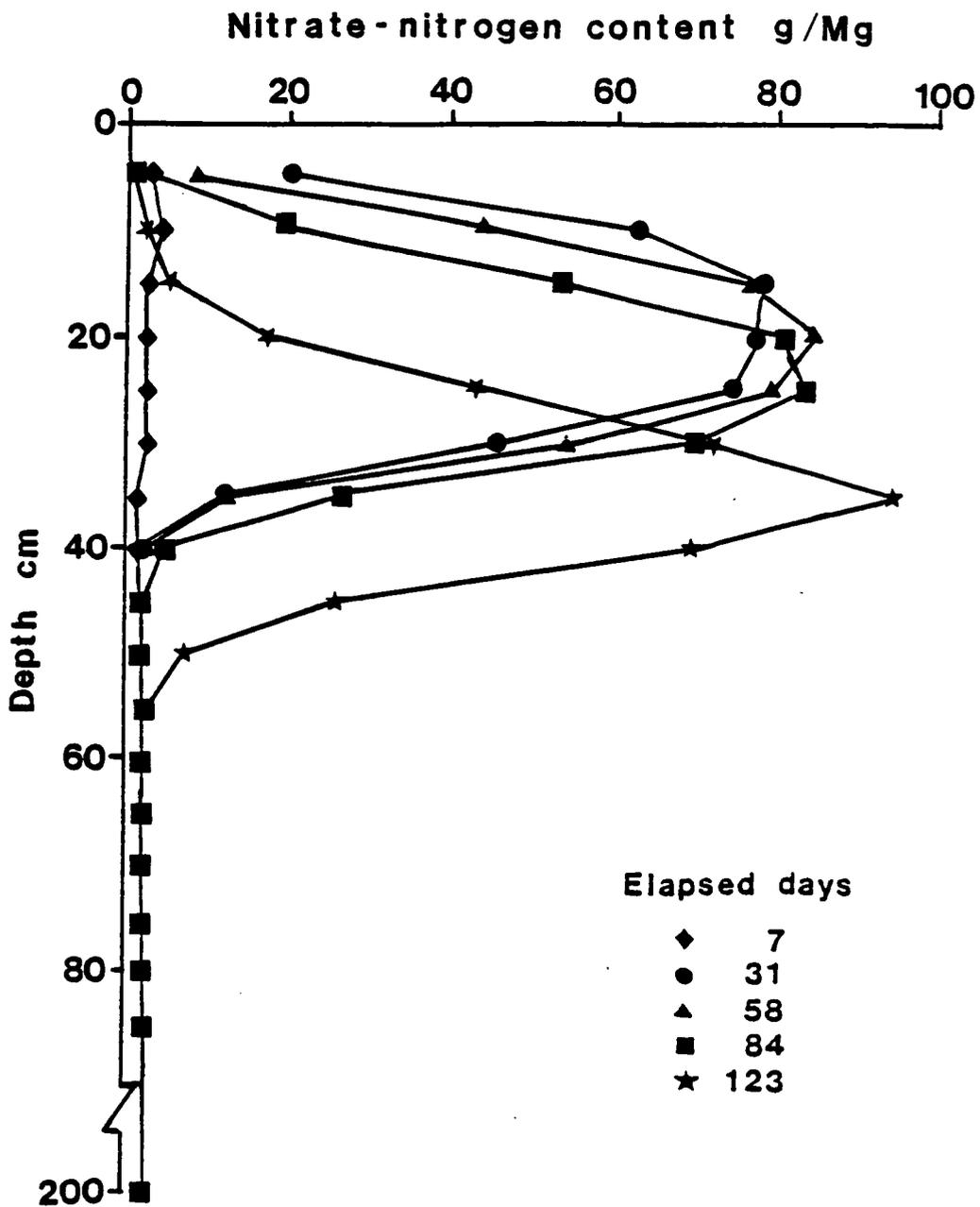


Figure 18. Changes in Nitrate-Nitrogen Profile with Time Following the 2-D Approach

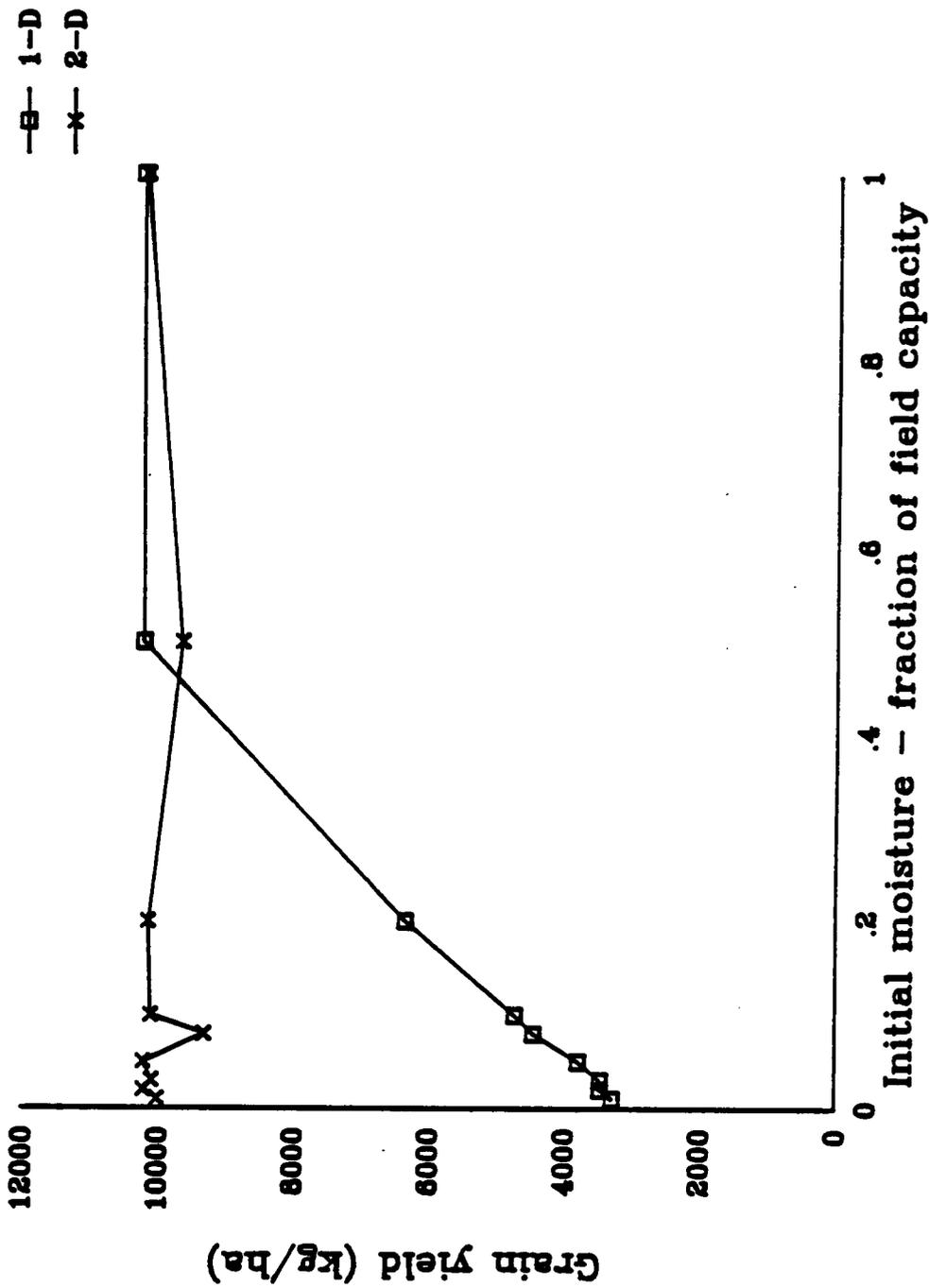


Figure 19. Grain Yield Variation Due to Varying Initial Moisture Contents

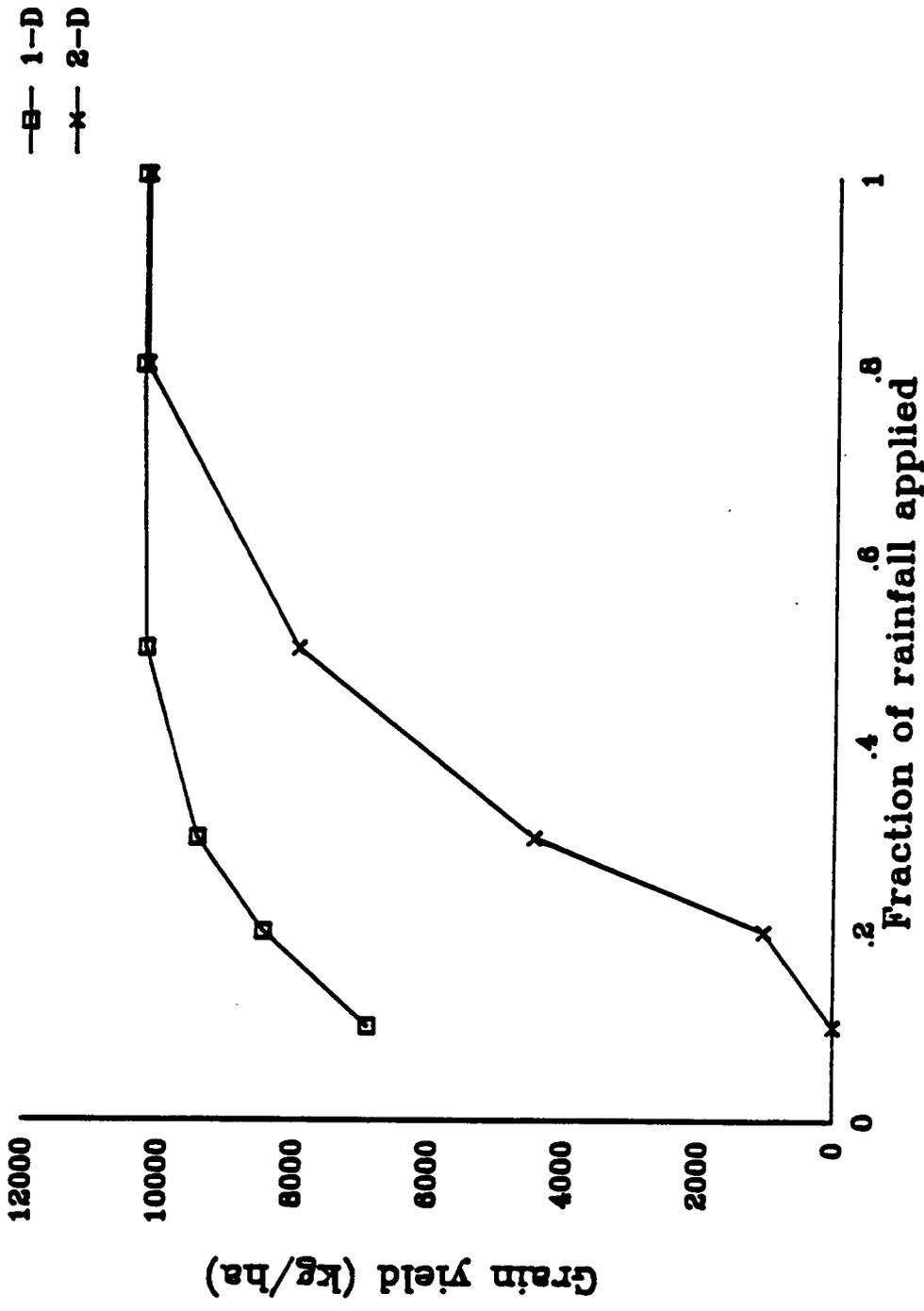


Figure 20. Grain Yield Variation Due to Varying Rainfall

buted to the assumption in the 2-D model that the maximum rate of active nitrate-nitrogen uptake decreases exponentially with the age of roots. This assumption may not be valid for very young roots or the assumption may be growth stage dependent.

Calibration

Table 6 shows the results of simulated vs actual silking date and grain yield for each of the 3 varieties of corn under both the 1-D and 2-D approaches. These results show that either approach can be calibrated to predict the silking date and grain yield of a variety.

Preliminary Credibility Assessment

Table 7 gives the scores of the preliminary credibility assessment for each individual judge and the overall scores after the responses of the judges were weighted. The results indicate that all judges felt the 2-D approach was more credible than the 1-D approach.

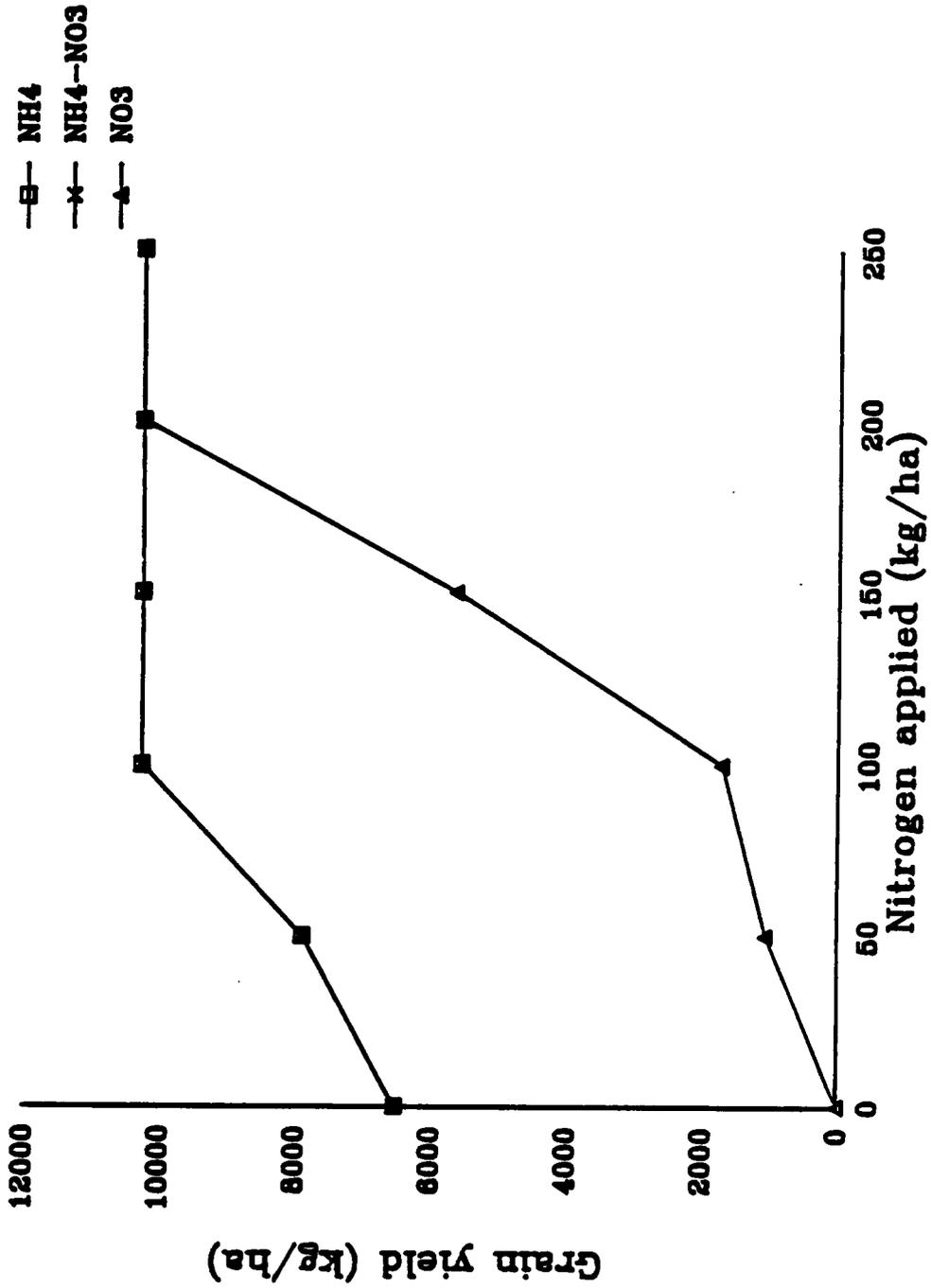


Figure 22. Grain Yield Variation Due to Varying Nitrogen Fertilization Practices Under the 2-D Approach

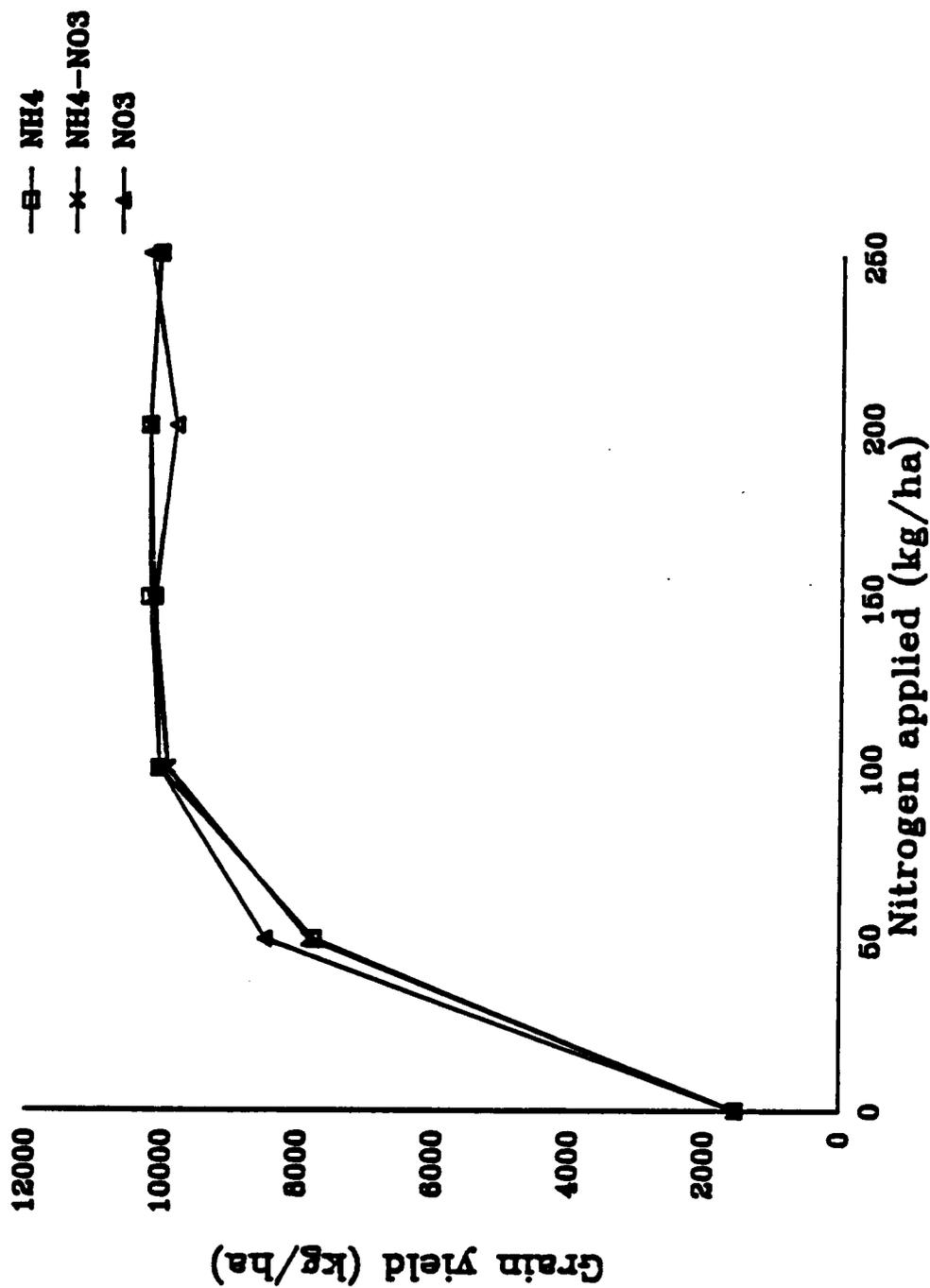


Figure 21. Grain Yield Variation Due to Varying Nitrogen Fertilization Practices Under the 1-D Approach

Table 6. Actual vs. Predicted silking date and grain yield after calibration for 3 varieties

Variety	Silking Date (calendar day)		Grain Yield (Kg/ha)	
	actual	predicted	actual	predicted
-- 1-D approach --				
Pioneer 3320	214	214	6343	6341
Pioneer 3744	207	208	6035	6081
Pioneer 3192	213	214	7221	7231
-- 2-D approach --				
Pioneer 3320	214	214	6343	6341
Pioneer 3744	207	208	6035	6081
Pioneer 3192	213	214	7221	7231

Table 7. Results of preliminary credibility assessment

Judge	1-D	2-D
SP	46.86	69.50
AC	91.80	91.90
PP	43.01	75.60
SA	85.27	99.10
Total weighted	66.71	83.99

Conclusions

Plant growth simulation under both the 1-D and 2-D approaches seems adequate. Plant growth and shoot:root ratios (Figures 8, 9, and 10) under both approaches follow expected trends and model calibration can be used to adequately predict crop growth (Table 6). More information is needed in the area of root growth. Root growth studies need to focus in the areas of varietal differences in the distribution of carbohydrates to root system and varietal differences in root respiratory losses of carbohydrates in order to adequately predict shoot:root ratios.

Soil nitrogen under both approaches follow expected trends. Both approaches simulate the expected changes in organic matter content (Figures 13 and 14), ammonium-nitrogen (Figures 15 and 16) and nitrate-nitrogen (Figures 17 and 18) over the growing season. However, there are differences between the amounts of ammonium-nitrogen and nitrate-nitrogen found in the soil system under the 1-D and 2-D approaches. Both approaches limit nitrification due to extremes in soil temperature and soil moisture however the 1-D approach uses an additional factor, called a nitrification capacity factor, to limit nitrification. This factor seems to overly limit nitrification and thus greater amounts of ammonium-nitrogen and lower amounts of nitrate-nitrogen are found in the soil. Studies are needed to quantitatively evaluate the levels of ammonium-nitrogen and nitrate-nitrogen in soil systems and the properties which limit the nitrogen transformation processes.

There are indications from these preliminary results that the 1-D approach does not adequately simulate soil water redistribution. First, the 1-D approach shows no movement of nitrate-nitrogen within the soil system (Figure 17) while the 2-D approach shows the expected advancement of a nitrate-nitrogen front within the soil system (Figure 18). Besides the stability of the nitrate-nitrogen front in the 1-D approach, the overly sensitive response of the 1-D approach to initial moisture content of the soil profile (Figure 19), and the relative insensitivity of the 1-D approach to rainfall variation (Figure 20) lead to the conclusion that the 1-D approach does not adequately simulate soil moisture redistribution.

The plant responds as expected to all nitrogen fertilizer applications under the 2-D approach (Figure 22) and to ammonium and ammonium-nitrate fertilization under the 1-D approach (Figure 21). The 2-D approach approach seems to slightly over estimate yields at the 50 and 100 Kg/ha application rates indicating that the assumption made that maximum root nitrogen uptake decreases exponentially over the entire growing season may not be entirely adequate and may be growth stage dependent. Further studies of the rate of uptake of nitrogen by plant roots need to be conducted. The high yield estimates of the 1-D approach when no nitrogen fertilizer is applied occurs due to the release of ammonium-nitrogen from the organic matter and the assumption within the 1-D approach that both ammonium and nitrate forms are taken up by the corn plant. The response of the 1-D approach to applications of nitrate-nitrogen is not fully understood and needs further investigation.

Overall, this preliminary evaluation of C-Maize VT1.0 indicates that the 2-D approach provides, at this time, a 'sufficiently credible' solution while the 1-D approach is 'not sufficiently credible'. The 1-D approach is insufficient due to the inability of the approach to redistribute water and nitrate-nitrogen within the soil subsystem, the overly sensitive response of the approach to the initial moisture specification, the insensitivity of the approach to additions of rainfall, and, finally, the inability of the approach to adequately simulate plant response to nitrogen. It is recommended that the 1-D approach be either eliminated or totally rewritten to follow the conceptualizations of the 2-D approach. Future work on the 2-D approach within the C-Maize VT1.0 simulation model

should include those areas already mentioned as well as field validation and a full scale credibility assessment.

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