1.1 Introduction and Research Perspective

Nitrogen has a key role in plant nutrition. Within the plant it is a constituent of amino acids which are utilized in protein synthesis. Many of the proteins formed in plant cells are enzymes and, as such, they control the metabolic processes that take place in plants. In addition to its role in the formation of proteins, nitrogen is an integral part of the chlorophyll molecule and is thus essential for photosynthesis. Nitrogen is the mineral element required in greatest quantity by cereal crop plants and it is also the nutrient most often deficient. As a result of its critical role and low supply, the management of nitrogen resources is an extremely important aspect of crop production (Novoa and Loomis, 1981).

The importance of nitrogen to crop growth has long been recognized and the use of nitrogenous fertilizers to boost crop yields has increased very substantially, particularly in the past 2 decades (Table 1). The importance of nitrogen fertilizer in

Table 1. Total Amount of Nitrogenous Fertilizer Consumed in Australia, the United Kingdom, and the World

Year	Australia[a] ('000 tonnes)	United Kingdom[b] ('000 tonnes)	World[c] (million tonnes)
1913	-	29	1.3
1939	-	61	2.6
1954	-	275	5.6
1960	-	330	9.7
1970	-	803	28.7
1975	335	980	38.9
1980	365	1,268	57.2
1984	387		70.5[d]

a. Anonymous, 1986.
b. Interpolated from Cooke (1982).
c. FAO (1981).
d. FAO (1986).

raising world grain yield during the past three decades is illustrated in Figure 1.1. The yield increases were obtained by exploiting the greater genetic potential of newer cultivars through the increased use of fertilizer and improved management. Hauck (1981) has estimated that fertilizer nitrogen is now applied to 11% of the earth's surface. Much of the expansion in fertilizer use in the past 2 decades has taken place in developing countries which consumed 40% of the fertilizer nitrogen used in 1980 (Craswell and Godwin, 1984). Nitrogen is currently the most widely used fertilizer nutrient and the demand for it is likely to grow in importance in the foreseeable future. The location and amounts of future N use will be determined primarily by the importance that developing countries place on increasing the production of food and fibre as well as by their success in real terms in improving the economic standards of the population (Stangel, 1984). Projections of growth in N fertilizer production and consumption (Figure 1.2), despite some current stagnation, further attest to the greater importance N will play in crop production in the future. Estimates of global N demand of about 90 million tonnes by 1990 and between 111 million tonnes and 164 million tonnes by 2000 have been reported by Stangel (1984).

Wheat is the world's most important cereal crop with about 500 million tonnes produced annually. It has a general adaptation of its photosynthetic and growth processes to daily mean temperatures in the range of 10°-20° C (Fischer, 1983) and is thus grown commercially in locations stretching from 55° N in the U.S.S.R. to 40° S in Australia and Chile. Wheat is generally not grown in the lowland humid tropics (<25° latitude) although crops may be found in the Sudan, India, Mexico, and Peru and in the high altitude areas of the low latitudes.

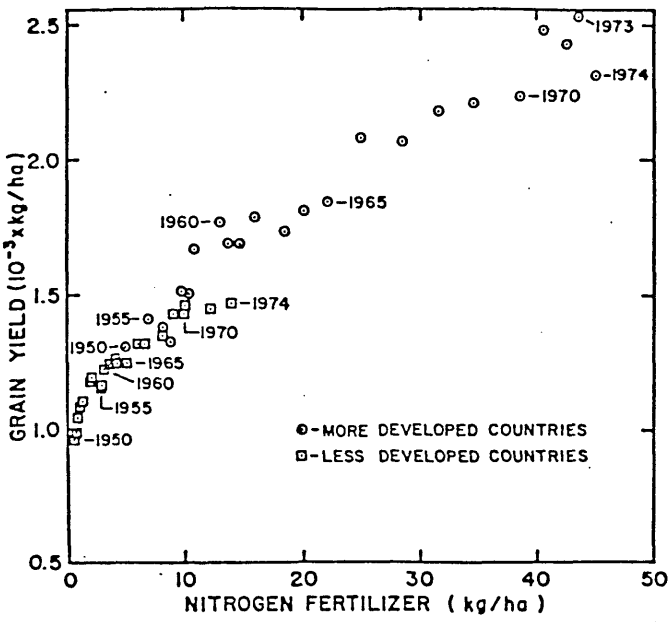

Figure 1.1 Relationship Beween Cereal Grain Yield and Rate of Nitrogen Fertilization Over the Period 1950-75. The Nitrogen Fertilizer Rate Was Assumed to be Half the Total Amount Used for All Purposes (After Hardy 1975).

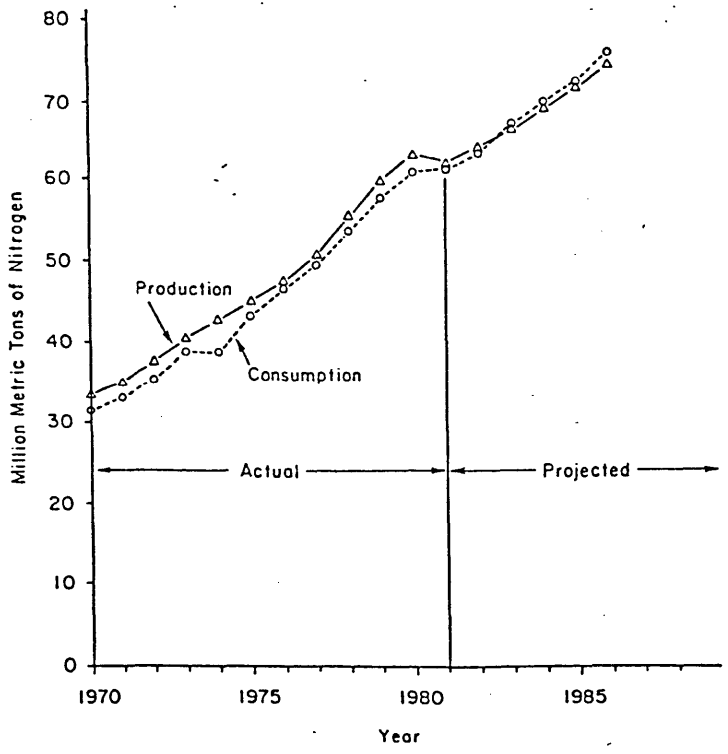

Figure 1.2. World N Production and Consumption. Actual 1970-80, Projected 1981-86 (After Stangel, 1984).

To enable wheat to span this great diversity of environments substantial genotypic diversity exists among cultivars. In European winter wheat-growing environments, wheat may often require as much as 11 months to complete the life cycle whereas short duration spring-planted spring wheats may require only 90 days to mature in the northern area of the wheat belt of North America. In the lower latitudes spring wheats are planted in the winter and the duration of the crop is from 3 to 6 months.

Crop growth, duration, yield, and fertilizer response are determined by environmental factors, plant genetic potential and crop management practices. The complexity of the various processes involved in the determination of yield and the response to nitrogen, as well as other environmental factors, makes it difficult to estimate yield and the magnitude of response to fertilizer.

Statistics compiled by Martinez and Diamond (1982) indicate that some 4.3 million tonnes of fertilizer N are applied to wheat annually. This survey did not include data from the U.S.S.R. and the People's Republic of China, two of the largest wheat producers. Using some assumptions based on current fertilizer consumption in these two countries (Harris, 1985), an estimated 8 million tonnes of fertilizer N are used annually for wheat. With the approximate energy conversion factor of 12 U.S. barrels of oil per tonne of fertilizer N (Mudahar and Hignett, 1982), this implies that the equivalent of 100 million barrels of oil is used each year to produce the fertilizer N for the world's wheat crop.

Despite the large investment in fertilizer nitrogen, the efficiency with which crops utilize it is poor. Allison (1965)

suggested the average recovery of fertilizer nitrogen in the above-ground parts of crops is about 50% and Power (1981) has indicated the general range of recovery in plant parts to be from 20% to 90% of the fertilizer applied.

The many different climatic environments in which wheat is grown have varying consequences for fertilizer use efficiency. In some of the more humid regions (e.g., Western Europe) fertilizer recovery is greatly influenced by the magnitude of nitrogen loss processes (leaching and denitrification) associated with periods of high water availability. Much of the world's wheat crop is grown in dryland areas, that is areas where the growth of the crop is periodically limited by a shortage of water. Under these circumstances fertilizer recovery may be adversely affected by short term drought preventing plant roots from absorbing nitrogen. This nitrogen not retrieved by the crop may either be lost from the profile during the noncrop period or remain in the soil for use by subsequent crops.

The nitrogen which is not recovered by the crop may be lost to the atmosphere through volatilization of ammonia or through denitrification of nitrate. Alternatively, nitrogen may be lost from the system by runoff or through leaching, or made unavailable to the plant through immobilization in the soil, or it may become inaccessible to the plant through lack of water. The magnitude of each of the various transformations affecting the use of nitrogen is influenced by many climatic, edaphic, and agronomic factors. The myriad of transformation pathways and the multitude of factors affecting transformation rates renders nitrogen as one of the most complex of plant nutrients to study. Quantifying these factors and predicting the response to added nitrogen is thus a very difficult task.

The fraction of nitrogen that is lost from the cropping system is a source of some of the environmental pollution associated with fertilisation. Thus for economic and environmental reasons a major thrust of current fertilizer research strategies is to improve the efficiency of its utilization.

Various attempts have been made to delineate some of the climatic factors affecting the efficiency of nitrogen use in differing agroclimatic zones (Russell, 1967; Craswell and Godwin, 1984). Reported data on fertilizer recovery, a common measure of fertilizer efficiency, are very variable both within and between agroclimatic zones (Craswell and Godwin, 1984) which compounds the difficulty of defining methods of improving fertilizer efficiency and crop yields.

Computer simulation models which are able to capture the nuances of weather and the effects of various soil properties and agronomic practices on nutrient dynamics and crop growth processes, potentially could make a large contribution to furthering our understanding of fertilizer behaviour and cropping systems. Such models, with the capability of readily simulating various crop and fertilizer management strategies, should lead to a great improvement in the efficacy of fertilizer decision making. Optimizing fertilisation strategies, given the uncertainties of climate, is generally difficult, and the problem is compounded in some less developed regions of the world where fertilizer data are sparse. Where adequate climatic, soil and crop data exist, simulation models will allow some extrapolation into these less developed areas and thus provide some insights into fertilizer behaviour in different environments.

The rapid advances in computer technology over the last two decades have meant that the computer is now a tool within reach of many agricultural researchers in the western world. The personal computer has also become a feasible acquisition of many developing country research institutions. These developments and advances in modelling have lead to the realization that modelling can greatly facilitate technology transfer. The IBSNAT (International Benchmark Sites Network for Agrotechnology Transfer) project (Uehara, 1984) is one such development which is designed to increase research efficiency through networking, systems analysis, crop modelling, and exploitation of these new wares of the information age.

Cooke (1979) recognized the role that models play in future research when defining priorities for British soil science. Bowen and Cartwright (1977), Penning de Vries (1981), Tejeda et al. (1981), and Myers (1986) have also highlighted the contribution modelling can make to fertilizer research. Greenwood (1981) has concluded that our ability to determine a response to fertilizer at the field level is currently "appallingly poor" and urges the development of more mechanistic approaches to being able to define fertilizer requirements for field crops.

To simulate N dynamics adequately in a range of diverse wheat cropping environments, a model capable of describing the major soil transformations, as well as the plant components, is required. The CERES-WHEAT-N model simulates growth, phenology, water and nitrogen balance, and yield, and it has widespread applicability in diverse environments.

1.2 Historical Perspective and Thesis Overview

The CERES-WHEAT-NITROGEN modelling project commenced in April 1981 as a collaborative effort between the International Fertilizer Development Center (IFDC) in Muscle Shoals, Alabama, and the Cropping Systems Evaluation Unit (CSEU) of the United States Department of Agriculture located at the Blackland Research Center in Temple, Texas. The basic aim of the collaborative agreement between the two institutions was to construct a model to describe the soil and plant processes which affect the response to nitrogen and the efficiency of utilization of fertilizer nitrogen in a diversity of environments where nitrogen is not present in optimal amounts.

In this thesis a consideration of the various modelling methodologies relevant to the problem of quantifying nitrogen fertilizer response and fertilizer use efficiency in diverse environments is presented in Chapter 2. Some of the limitations and deficiencies of various approaches to this problem used in the past are outlined. An overview of the systems approach is provided and a broad strategy for the development of a user-oriented computer simulation model of N dynamics in wheat cropping systems is advanced. The CERES-WHEAT model provided a sound base on which to construct a nitrogen model since it has been successfully tested in many diverse locations. This model and the development of the nitrogen components is discussed in Chapter 3.

During the course of development of the model, various data sets to test the complete nitrogen model were acquired. Details of test procedures and model performance are documented in Chapter 4.

One frequently encountered problem when using models of this type to quantify various crop and fertilizer parameters is the lack of sufficient long-term climatic records. This problem is addressed in Chapter 5 and a weather generator model to provide synthetic sequences of daily weather data is evaluated. Appropriate coefficients to enable generation of weather sequences for numerous locations in the Australian wheat belt are provided.

The sensitivity of the model to changes in the various input parameters is examined in Chapter 6. The appropriateness of certain key coefficients in major relationships is also tested in a further sensitivity analysis described in this chapter. Analyses of this type enable the modeller to determine how accurately certain parameters need to be measured and can also thus provide a valuable input into field programs.

Grain yield, fertilizer recovery, and the processes affecting them vary greatly from year to year in any location. Thus, to develop optimal fertilizer strategies in any location, it would be desirable to have fertilizer experiments conducted over many years. Since these data are seldom available, simulation of time series can provide valuable insights into temporal variability. Chapter 7 introduces the concept of analysis of temporal data generated when the model is coupled to the weather generator described in Chapter 5. Cumulative probability functions are generated for grain yield, N uptake, fertilizer use efficiency, fertilizer recovery, and for the various loss process. An examination of the consequences of various fertilizer strategies in differing wheat-growing environments is made in Chapter 7 and ideas on how to improve the efficiency of fertilizer use are advanced.

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On a religion for model builders (Van Dyne and Abramsky, 1975):

(i) They are devout, their faith is unwavering; almost certainly, they are more devout than sane agriculturalists. They are imbued and driven by the faith that even though the approach may not have worked yet, it remains one of the few paths to truth and light!

(ii) They hold perhaps more faith than many agriculturalists in absolutes, in ubiquitous patterns, universal principles, or natural laws. But agricultural modellers seek these grails in only an abstract and generalised sense. Further, they have unshaking faith in the model builders' ability to abstract such universals.

(iii) In seeming contradiction to his acceptance of generalised agricultural principles, the model builder generally does not believe that he cannot test these principles, or conclusively prove their existence. He recognises that his faith is pure and untainted by statistical exercise. He may state that "the model is of most use when it is clearly wrong."

(iv) Although supported by an imperturbable faith in general patterns, the model builder is convinced that only a small portion of the elements and patterns within a system are important (as opposed to the agriculturalists' teleological view). In the face of Pascal's statement that "error comes from exclusion" the modeller believes that "error comes from inclusion." He adopts the teleological view of nature to the extent of recognising basic patterns, but remains convinced that there is a lot of garbage lying around with no real purpose--

"noise" in the jargon of a communications engineer--containing little information.

(v) An outcome of these combined feelings is that the model builder assumes pattern through time and relative magnitude to be more important than absolute magnitude.

2.1. Systems Simulation and Modelling Overview

2.1.1. Systems

A system is a limited part of reality that contains interrelated elements, a model is a simplified representation or analogue of a system and system simulation may be defined as the art of building mathematical models and the study of their properties in reference to those of systems (de Wit, 1982). Systems can be defined in terms of their components and their boundaries.

Dent and Blackie (1979) define a system as having the following general features:

1. A system is fully defined both by a set of identifiable entities (or components) and interconnections between them and by the limits to their organizational autonomy.
2. A system is a hierarchical structure comprising a number of subsystems each capable of autonomous definition; in turn, subsystems similarly embody the next layer of detail in autonomous sub-subsystems. The point of entry into the hierarchy in any systems study is related to the objectives for which the system is being studied. The number of layers of the hierarchy included in any study will depend on the judgment of the researcher, but certain rules of thumb will be established.
3. The most important characteristics of systems emerge over time so that the understanding of systems requires explicit consideration of time and rates of change.
4. Systems are sensitive to the environment in which they exist. This environment is usually unpredictable and certainly variable.

Each of the components of the system can be further resolved into smaller components and new boundaries defined. A hierarchy of subsystems, in which one level of system is nested within another, thus exists as depicted by France and Thornley (1984) below:

Level	Description of Level
i + 1	Collection of organisms (herd, flock, crop)
i	Organism (animal, plant)
i - 1	Organs
...	Tissues
...	Cells
...	Organelles
...	Macromolecules

Each level encompasses the behaviour and mechanisms of the subsystems of lower levels. Thus a description of the behaviour of the system at level i can provide an understanding (either mechanistically or by explanation) of phenomena occurring at level i + 1. In order to simulate the behaviour of the system at level i, a model should have components describing mechanisms at level i - 1 and this in turn should describe mechanisms at level i - 2 and so on. Obviously there comes a point when a model becomes very complex if all of these subprocesses are included. In practice, in model building deficiencies in knowledge are soon encountered which should define the level at which systems are modelled; often whole subsystems may be either only poorly described or poorly understood. Description of these subsystems

is then either not included or entered as a "black-box" (van Dyne and Abramsky, 1975) and the model of the whole system is then often only as good as the weakest component (France and Thornley, 1984). Models should thus be constructed at the level of data availability.

Much of the impetus for the increasing interest in and development of models in the agricultural sciences has stemmed from our increasing insights into biological processes, the desire to optimize production, and concerns about global food production. This has spurned a consequent need for tools to synthesize and summarize knowledge. Advances in the computer industry placing the computer within reach of more agricultural scientists have stimulated this interest by making the tool potentially more available. There are many reasons why modelling should be considered as an adjunct to traditional research. Thornley (1976) has listed some of these as:

a. A mathematical basis for hypotheses enables progress to be made towards a quantitative understanding of plants and their response to environment.

b. An attempt at model construction can often help in pinpointing areas where knowledge and data are lacking.

c. Modelling can stimulate new ideas and experimental approaches.

d. Modelling may lead to a reduction in the amount of ad hoc experimentation, enabling the design of experiments which answer particular questions and discriminate between alternative hypotheses.

e. Compared with traditional methods, models often make better use of data, which are becoming increasingly precise but more expensive to obtain.

f. Information on different aspects of plant growth can often be brought together, giving a unified picture, and sometimes providing a valuable stimulus to collaboration and teamwork.

g. A convenient data summary is frequently provided by a model.

h. Models can give a method for interpolation, extrapolation, and prediction.

i. A successful model may be used to suggest priorities for applied research and development and, if used cautiously, to aid the crop manager in taking decision.

2.1.2. Types of Models

A static model is one that does not contain time as a variable (France and Thornley, 1984). Because all elements of biological systems vary with time, static models of the N cycle are only approximations (Myers, 1986). Models which describe variation with time are termed dynamic models. These are often expressed in a differential equation form, e.g.

$$dy/dt = f(x)$$

or alternatively in a finite difference form:

$$y = y0 + bT$$

where:

y0 is the output at time 0.

t is the unit of time.

and b is a constant.

Most recent models of N behaviour in soil-plant systems are dynamic and consider inter-relationships of factors that vary with time.

Models can also be classified according to the type of information generated by them. Deterministic models produce information only on the mean response of the real system to a change in one of its variables (Dent and Blackie, 1979). Stochastic models, in addition to predicting the response of the system to a change in one of its variables, provide some information on the probability of this outcome. The models described in this Chapter and in Chapter 3 are deterministic and those described in Chapters 5 and Chapter 7 are stochastic. Further description of stochastic models may be found in Mihran (1972) and Dent and Blackie (1979).

When developing a system simulation model, various methods may be used to construct the individual components. The approach used largely reflects the preference of the individual modeller, the purpose for which the model is being constructed, and data availability. Existing models may be broadly categorized as:

1. Empirical models in which a description of the system is provided without necessarily providing an understanding of that system. In this approach, equations are fitted to data sets by regression analysis, so that any given variable can be estimated from one or more other variables (Myers, 1986). Such models can be used as predictive tools provided the goodness of fit is satisfactory and some caution is exercised. The note of caution is necessary because the fundamental assumption of an empirical model is that underlying mechanisms do not change from situation to situation.
2. Mechanistic models which are constructed by looking at the structure of the system, by dividing the system into components, and by trying to understand the behaviour of the whole system in

terms of the behavior of the individual components and their interactions with one another (Thornley, 1976). Mechanistic models can be used predictively provided the description of the necessary mechanisms is appropriate.

These two types of models are not always distinct, and many modellers have used an intermediate or combined approach to the two. Thornley (1976) defined this intermediate approach as a phenomenological approach which has an approximate mechanistic description or an empirical approach with a strong flavour of mechanism. Some examples of the phenomenological models used in crop physiology cited by Thornley are: a rectangular hyperbola for a description of leaf photosynthetic response to light and carbon dioxide concentration, a Michaelis-Menten relation for describing the substrate dependence of complicated processes such as growth and respiration, and the description of transport phenomena by a concentration difference divided by a resistance.

Stapper (1984) in a review of modelling methodologies defined another approach intermediate between a fully empirical and a phenomenological one. He termed this a correlative approach in which regression or other statistical techniques which describe theoretical relationships between elements are used. The weather simulator models described in Chapter 5 are of this type. Generally, model complexity and the number of parameters utilized increases as one proceeds from an empirical model to a fully mechanistic model. Stapper (1984) examined these four different approaches to categorize crop models. By analogy with his categorization, models describing the response of a crop to N can be similarly categorized as follows:

1. Empirical response models in which crop yield is simply related to the amount of fertilizer applied.
2. Response-weather-soil test models. Extensions to the simple response model are provided to describe such factors as initial levels of soil fertility and seasonal rainfall.
3. Crop-growth response models. These models are dynamic and incorporate components to describe plant growth as it is affected by N supply and possibly weather. Water use and soil transformations are modelled using mainly correlative or phenomenological relationships.
4. Crop-soil-system models. These models incorporate components to describe crop growth, water balance, and nutrient transformations all at approximately the same level of detail.
5. Process-oriented models. These models describe nutrient transformations at the process level often with description of the microbiological phenomena involved. Some models describe only selected transformations while others attempt to describe the whole system at this level.

Figure 2.1 provides a summary of the characteristics of these five categories. The different approaches to modelling are discussed in the following sections.

2.1.3 Procedures of Model Building

Systems simulation has two fundamental components. The first of these involves the construction of a model and the second involves

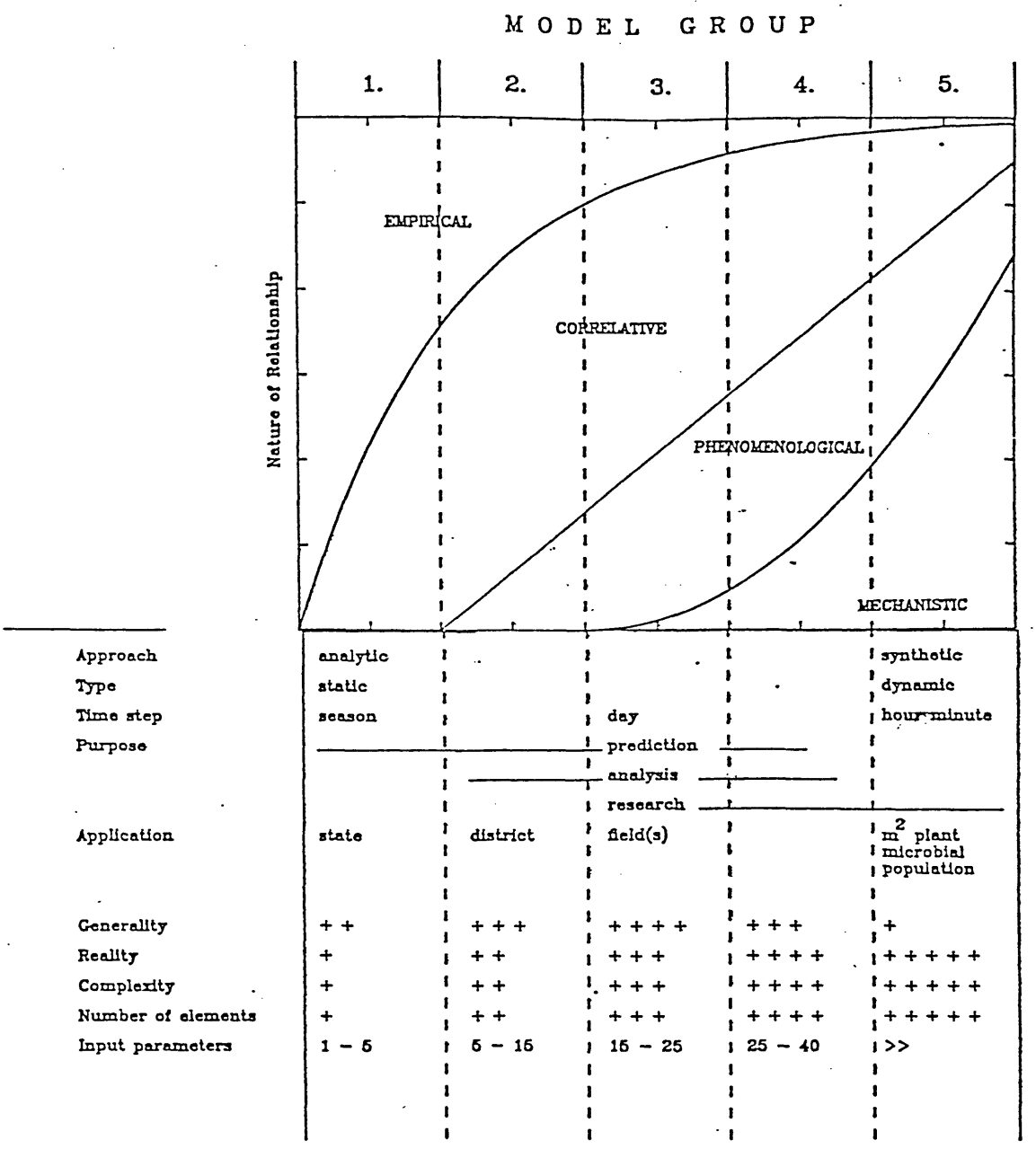

Figure 2.1. Schematic Presentation of the Nature of Model Content for Five Types of Model Which Describe Response to Fertilizer and a Summary of Model Characteristics.

Model groups are:

1. Empirical Response Models.
2. Response-Weather-Soil Test Models.
3. Crop-Growth Response Models.
4. Crop-Soil System Models.
5. Process-Oriented Models.

(Adapted from Stapper, 1984).

application of the model in addressing the problems related to the real system. These components may be resolved into several smaller steps which are interlinked. Dent and Blackie (1979) have summarized these basic steps in model building and their interlinkages (Figure 2.2). The structure described here provides a broad overview of systems thinking and methodology. The various steps depicted in the diagram form a framework for the following chapters of this thesis.

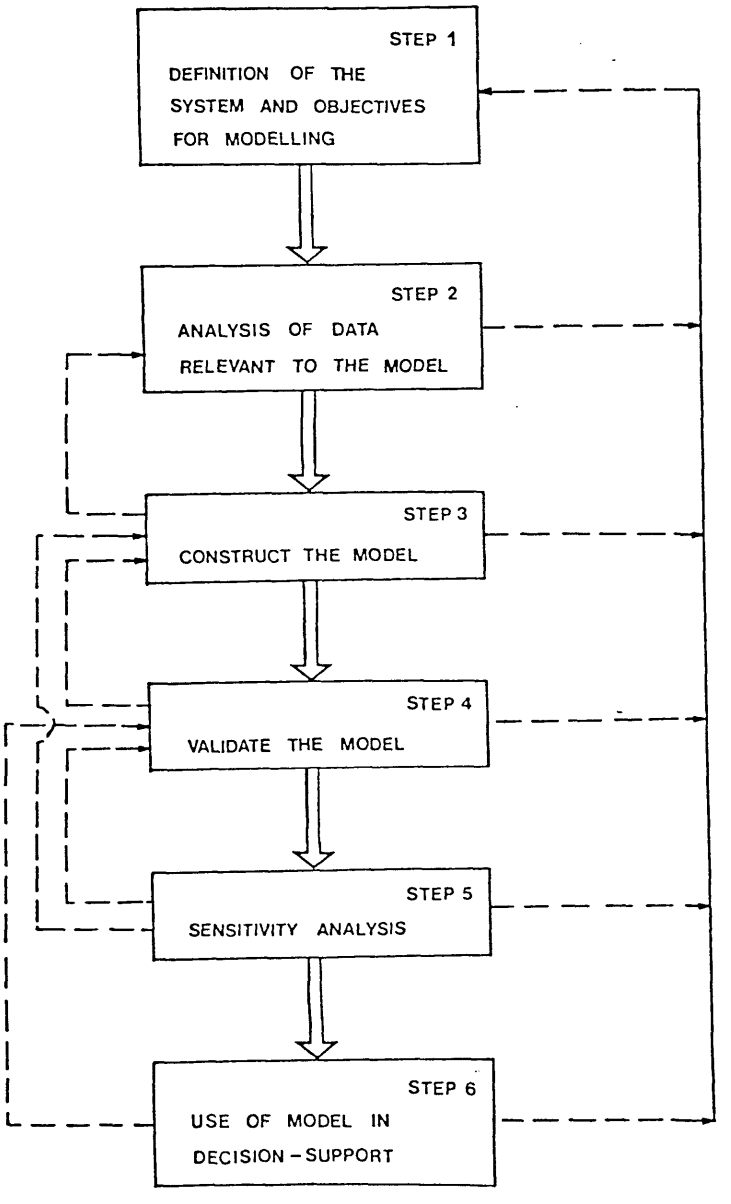

Figure 2.2. The Basic Steps of Systems Simulation (From Dent and Blackie, 1979).

2.2. Fertilizer Response and Response-Weather Models

When farmers apply fertilizer they face a decision as to how much fertilizer to apply and to enable them to make this decision some knowledge of the likely response is required. Traditionally, information to generate a response curve is obtained from field experiments that test several increasing dressings of each nutrient to show how the fertilizer affects crop yields. This response information then forms the basis for deciding an optimum amount to apply.

If this response can be numerically quantified, the biologically optimum amount of fertilizer to apply can be obtained from simple calculus procedures. Economic optima similarly can be obtained from a response curve described in terms of profits and cost. The desire to find optima has thus rendered response analysis a major preoccupation of biometricians and agricultural economists over the last century.

Early work by Mitscherlisch (see Tisdale and Nelson, 1975) in the 19th century led to the first quantification of response to added nutrients. The work led to the development of an equation which related growth to the supply of plant nutrients. Mitscherlisch expressed this mathematically as

$$dy/dx = (A-Y)C$$

where:

dy is the increase in yield (Y) resulting from an increment (dx) of the growth factor X.

A is the maximum possible yield obtained by supplying all growth factors in optimum amount.

Y is the yield obtained after any given quantity of the factor X has been applied.

C is a curvature coefficient dependent on the nature of the growth factor.

An alternative expression of this function commonly used in fertilizer response studies is:

$$Y = A(1-e^{-cx})$$

Various modifications to the basic functional form have been made to accommodate responses to more than one growth factor (Tisdale and Nelson, 1975) and to account for the residual value of previous applications (Helyar and Godden, 1975). Further evaluation and modification of this function has been carried out to account for differences in mobility of different ions (Balba and Bray, 1957; Russell, 1971). A third coefficient "B" is often added to the function to account for the ability of a particular soil to supply a nutrient. It has also been used to help define the residual value of a previous application of fertilizer (Bowden and Bennett, 1974).

The modified functional form then becomes:

$$Y = A(1-Be^{-cx})$$

However, the Mitscherlisch function is asymptotic (see Figure 2.3) and thus cannot be applied to the full range of responses when the response is parabolic as often occurs with responses to nitrogen (Cooke, 1982). Since the shape of the response can vary greatly depending on the circumstances, numerous other functional forms have been utilized to describe the response to fertilizers. Among these are:

1. Square root function (FAO, 1966).
2. Hyperbolic function (Campbell and Keay (1970), Hagin (1960).
3. Cobb-Douglas power function (Heady and Dillon, 1961).
4. Resistance function (Freitas et al., 1966).
5. Transcendental function (Rao et al., 1965).
6. Logistic function (Smith, 1976).
7. Polynomial function (Dillon, 1968; Colwell, 1978).

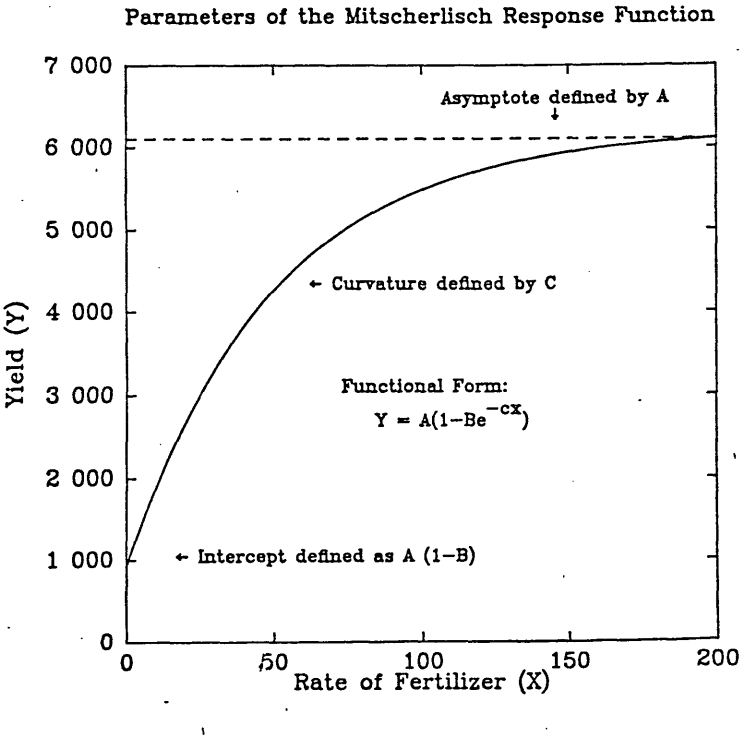

Figure 2.3. Schematic Representation of the Mitscherlisch Response Function.

Depending upon the nature of individual data sets each function may have certain advantages or disadvantages. No standard equation is unilaterally acceptable which is an acknowledgement of the fact that fertilizer response curves have no standard form, but their shape depends also on the crop and nutrient and on local conditions

of soil, weather, and farming methods (Cooke, 1982). Of those listed the most commonly employed is the polynomial which offers the advantages of:

1. Ease of fitting the equation to data with least squares regression methods.
2. Statistical error analyses of estimates can be performed on the function and their significance tested.
3. The function lends itself readily to calculus procedures used in the determination of optimum rates of fertilizer.

Marked variations in fertilizer response can and usually do occur from period to period and from location to location or from region to region when experiments are replicated over space and time. The chief causes of this variation are differences in climate and soil properties and especially initial soil fertility levels.

Various methods of modifying response curves to enable them to accommodate some of these factors have been attempted. A common approach has been to incorporate the effect of differences in initial soil fertility by manipulating the functional form to describe the response to fertilizer in terms of both amount of fertilizer added and an initial soil test value which provides an estimate of the amount of nutrient present. Usually this is accomplished by an adjustment to the intercept terms. Procedures for estimating the appropriate coefficients to add to polynomial response functions when soil test data are available have been developed (Voss and Pesek, 1962). Bray (1944) proposed a modification of Mitscherlich's fertilizer response model in order to accommodate soil test values to describe the response to phosphorus. Black (1955) extended this

modification further by utilizing a linear combination of soil test values taken at different depths and representing different availabilities of the nutrient. This combination was used to adjust the shape of the Mitscherlisch. Similarly, Bowden and Bennett (1974) have used the "B" coefficient of the Mitscherlisch equation to adjust for residual values of past phosphate applications in the "DECIDE" model. The DECIDE model also utilizes various soil properties and an arbitrarily defined local area maximum to determine the response to phosphatic fertilizers.

Because the response curve is static in nature none of these procedures can effectively be used from season to season or in regions other than that which was used to characterize the response. Various approaches have been adopted to render a response curve less location- and time-specific. This is of particular relevance when describing the response to nitrogen fertilizer since a great diversity of responses can occur. The modifications generally have involved addition of extra terms in multiple regression equations to describe soil properties and certain climatic factors. A summary of some of the modified models used to describe the response to N is tabulated below (Table 2.1). These indicate the available water supply and the ability of the soil to supply nitrate as major determinants of response. Many of the studies included total growing season rainfall or rainfall over shorter periods but rainfall distribution within a period, which is often a more important yield determinant than total rainfall, is not considered.

In all of these cases it can be seen that the variance accounted for by the functions, though significant, is not large. While models

Table 2.1. Summary of Some Multiple Regression Models Relating Yield or Nitrogen Requirement of Cereals to Soil and Climatic Factors

Reference	Location	Crop	Dependent Variable	Variables Used	$100R^2$
Young et al. (1967)	North Dakota, United States	Spring wheat and barley	Yield	ASM, GSP, OCV, NO_3	49.7
Jackson and Sims (1977)	Montana, United States	Winter wheat	Yield	NO_3, OCV, GSP, NMI	43.3
			N fertilizer requirement	NO_3, Y, GSP, ASM	58.1
Heapy et al. (1976a,b)	Alberta, Canada	Spring barley	Yield	FR, NO_3, EP, OMI	57.0
Taylor et al. (1974)	New South Wales, Australia	Winter wheat	Yield	OMI, GSP, NO_3, OAF	61.3
Taylor et al. (1978)	New South Wales, Australia	Winter wheat	Yield	GSP, OAF, NO_3, NMI	42.3
Russell (1968a)	South Australia, Australia	Winter wheat	Yield	GSP, NMI, NO_3	48.1
Russell (1968b)	South Australia, Australia	Winter wheat	Yield	GSP, NO_3	46.5

ASM = available soil moisture at sowing.
GSP = growing season rainfall.
OMI = other moisture indicators.
OCV = other climatic variables (e.g., temperature, evaporation).
Y = grain yield.
NO_3 = soil nitrate at sowing.
NMI = N mineralization index.
EP = extractable soil P.
FR = fertilizer requirement for maximum yield.
OAF = other agronomic factors (e.g., sowing date, seeding rate, weeds).

Adapted from Myers (1984).

of this nature may adequately describe a set of data, their use as predictive tools is limited by the variables included, the range of values the variables take and by the interactions of the variables within this range. The models are restricted to the geographical region or range of climatic conditions under which they were developed and are specific for the crop type and crop management practices used.

These limitations appear to have led to attempts to incorporate other terms in models or to approach the problem differently. For N, one approach has been to calculate the ability of the soil to supply N to the crop and to deduct this from the crop's requirement to produce a prescription for the amount of N required. The N response of the crop is partitioned into the components of N demand, N supply, and the efficiency of N uptake. Stanford (1973) has developed a static model which incorporates the N requirement for "attainable" yield, N mineralized during the cropping season, residual mineral N, and the efficiency of uptake. A "balance sheet" approach similar to this has also been proposed by Remy and Viaux (1982) and Remy (1985). Ostergaard et al. (1985) utilized a similar approach, but included an allowance for leaching. All of these methods assume some a priori knowledge of the potential yield. They do not consider seasonal effects on crop growth and hence demand for N, nor do they consider seasonal effects on N supply processes. Use of this method to determine optimum amounts of N to apply has thus largely been confined to areas of intensive agriculture with a relatively small degree of climatic variability such as some of the wheat-growing areas of western Europe. The models are not designed to describe a response to fertilizer, but to provide a prescription for fertilizer amount.

Myers (1984) has developed a similar model but has attempted to make it less site- and season-specific by including parameters to describe the effects of soil water supply on both the N supply processes and the N demand components. The method requires estimation of a potential yield based on stored available soil moisture at planting (WST) and total rainfall during the growing season (WRF). The N required to achieve this potential yield (N_{max}) is determined from a linear relation with yield. The fertilizer requirement (N_{fert}) is then calculated from the balance of supply and demand allowing for the efficiencies of uptake:

$$N_{fert} = \frac{1}{Eff_2} (N_{max} - N_{sup} \cdot Eff_1)$$

where:

Eff_1 = the efficiency of uptake of soil mineral N (estimated as a function of WST and WRF).

Eff_2 = the efficiency of uptake of fertilizer N (defined as 80% of Eff_1).

N_{sup} = the N supplied by the soil which is calculated as the sum of the soil mineral N and the N mineralized during crop growth.

The N mineralized during crop growth is estimated from the total soil N, WRF, and latitude.

The validity of the model depends greatly on the accuracy of the estimates of soil N supply and potential yield. Since both of these are determined from total seasonal rainfall with no consideration of rainfall distribution, the estimates will be very crude. Tests of

the model (Figure 2.4) for winter grown wheat in Australia and the United States indicate the estimates of N_{fert} are frequently poor. In regions with even less climatic variability such as the United Kingdom, methods of determining N fertilizer requirement based on mineralizable N have performed poorly (Needham, 1982).

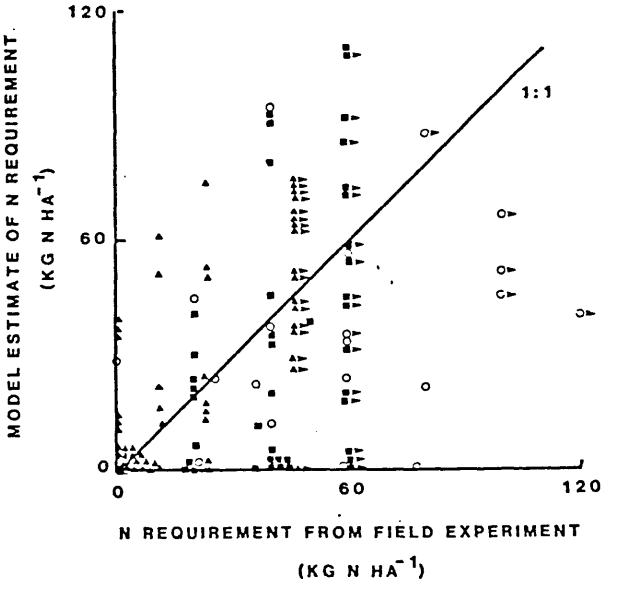

Figure 2.4. Tests of the Myers (1984) Model for Winter Wheat Using Data From Nebraska (●), Kansas (o), and South Australia (▲). Symbols ▶ Refer to Trials Where the Response Curve Appeared not to Have Reached a Maximum. (From Myers, 1984).

Alternative methods of determining N requirement which rely upon early stage plant analysis for total nitrogen (Moller-Nielsen and Friis-Nielsen, 1976) have also been suggested, but in many cases these have also performed poorly (Needham, 1982) possibly because by the time deficiency can be diagnosed from tissue analysis substantial loss in potential yield may already have occurred.

Xylem sap nitrate content has also been used as a diagnostic criterion to indicate when fertilizer should be applied (Papastylianou, 1982; Darby et al., 1986). Methods of determining optimum amounts of fertilizer to apply based on this diagnostic criterion rely on the assumption that a relationship between tissue concentration and yield always holds. Although providing a prescription for amount and timing of fertilizer applications, the method cannot provide quantitative information on response to N.

While approaches such as those of Myers (1984) add more generality to describing fertilizer responses than traditional multiple regression models, the models are still static in nature and are unable to account for within-season variability in the supply of either water or nutrients. Although the approaches described above are simple to generate and are readily adaptable by economists for determining economic optima, they are not suitable for extrapolation from season to season or from site to site. Regression analyses, while providing correlations between certain variables, do not test any theories about the mechanisms involved, although they may suggest where theories are to be sought (Nye et al., 1975). Dynamic models which accommodate the effects of weather, soil type, and crop and management effects promise to overcome many of these shortcomings of the regression approach.

2.3. Crop Growth Response Models

These models differ from the static models described above in that they try to simulate the daily growth of a crop in response to its aerial and soil environment. In principle it should be possible

to account for yield and response variations from year to year as well as the effects of management with these models.

Dynamic models which describe the daily growth rate of the crop as affected by N supply have been developed for sugar beet (Greenwood et al., 1984), potatoes (Greenwood et al., 1985), and lettuce (Greenwood et al., 1974). These models are designed for fertilizer recommendation purposes in the vegetable growing areas of the United Kingdom. The models estimate growth by first calculating a duration of growth (based on crop weight) and then determining a potential increment of crop growth for each day. Actual crop growth is determined in each case by assuming a logistic growth function, and modifying the growth rate according to the prevailing N status of the plant. The salient features of the potato model are:

Crop Growth--A maximum potential dry matter increment (Δw in t/ha) which can occur over time Δt is calculated:

$$\frac{\Delta w}{\Delta t} = \frac{K_2 W}{K_1 + W}$$

where:

W = weight of dry matter (t/ha).

K_1, K_2 are coefficients.

The actual increment in dry matter production is the product of this potential and a growth factor (G_f). This growth factor is calculated as a ratio of a actual plant N concentration (P_w) and the minimum plant N concentration where growth is at a maximum (P_m) and the concentration where growth ceases (P_o).

$$G_f = (P_w - P_o)/(P_m - P_o)$$

A function is incorporated which allows P_m to decline as the crop grows. Thus crop growth rate is reduced only by the N deficit effects.

Mineral N Supply--The model assumes a constant daily rate of mineralization and calculates redistribution of inorganic N throughout the profile using the leaching model of Burns (1974).

Root Depth--Root penetration increases roughly linearly with increases in plant weight until a stage is reached where no further penetration occurs.

N Uptake--A potential maximum uptake is calculated as the product of the potential maximum increment in dry matter and the maximum possible % N in the dry matter. This maximum possible % N is set at $1.2 \times P_m$. Actual N uptake is calculated from this maximum potential uptake, the amount of available N to the depth of rooting and a recovery fraction FR. This is modified according to the proportion of the cross-sectional area of the soil which is exploited (which in turn is estimated as a function of plant weight). The model has no water balance component, and the effects of soil water and rooting density on nitrogen mobility and uptake are ignored. Inorganic N is firstly removed from the surface layer and then from the next layer and so on down the profile.

Partitioning of N and Dry Matter Within the Plant--The partitioning of dry weight and N between tops and tubers were calculated as time dependent functions.

The sugar beet and lettuce models are similarly structured. These models offer the advantage of simplicity and require few data to run them. They have also performed well in the testing conducted by the authors. This testing, however, has been confined to data sets

from the experimental stations where the models were developed and has thus not received independent testing from a diversity of independent data sets. The approach adopted in the models unfortunately has several serious shortcomings for use in a crop model of global applicability. Some of the assumptions implicit in the models which are not valid beyond the locations where they were developed are:

1. A constant monthly solar radiation over the growth period.
2. Growth duration is determined as a function of the final biomass.

   In determinant crops growth duration is independent of harvest biomass and is a function of environmental and genetic factors. The approach used by Greenwood et al. will not apply in environments where stresses (temperature, light, water, and nutrients) will affect the assumed relationship between duration and biomass.
3. The N mineralization rate in soils will differ greatly in soils from region to region and since mineralization rate is dependent upon temperature and moisture will differ from season to season. Under conditions of low N supply (unlikely under intensive vegetable farming conditions) assuming a constant rate of mineralization will lead to errors in the estimation of N supply to the crop.
4. The depth of rooting is assumed constant and is thus not sensitive to soil properties which may influence this in other environments.
5. The model does not consider a limitation on growth or N uptake imposed by soil water constraints. Clearly in most rainfed environments this will greatly limit applicability.
6. The model assumes N losses from the soil are zero. N losses occur frequently and can be substantial (Power, 1981).

7. The effects of other stresses, notably temperature and water on growth and yield are not considered.

These models, while providing reliable and valuable information enabling fertilizer recommendations to be made, are highly location specific and cannot be used with confidence outside the region of their development. The models also do not consider the effects of plant population, time of sowing, or varietal differences in growth and response to fertilizer nor do they consider the effects at varying fertilizer management practices.

Models which can provide greater generality and which can be used in a diversity of environments may require more complexity. To provide greater generality, models require adequate description of how crop growth and nutrient supply processes are affected by the environment. Several crop models which meet this criterion of being able to operate in a diversity of environments have been developed. Some of the more recent models for cereal crops and a listing of the processes they describe and the modelling approach used are tabulated below (Table 2.2). In all cases with the exception of the United Kingdom wheat model (Weir et al., 1984), a water balance forms part of the model. Approaches to growth and development simulation differ between models. A more detailed description of these various approaches is beyond the scope of this thesis, but may be found in Stapper (1984) and in a recent book (Hanks and Ritchie, 1987).

Of the models tabulated only the CERES models (Ritchie et al., 1987; Jones and Kiniry, 1986; and Ritchie et al., 1986) and the rice model of Angus and Zandstra (1980) simulate the processes of crop growth and development as well as including a component describing

Table 2.2. Some Published Dynamic Simulation Models for Cereal Crops

Crop	Submodels								Environmental Factors	Reference
	Phot	Nutr	Part	Transp	Gr & R	LA exp	Dev	Sen		
Barley	mech				mech				I,W,T	Legg et al. (1979)
Maize	mech	emp	emp	mech	mech	emp		emp	I,W,T	de Wit et al. (1978)
Sorghum	mech	emp?	emp?	mech	mech	emp	emp		I,W,T	Arkin et al. (1976)
Wheat	mech	mech	mech	mech	mech	mech	mech	mech	I,W,T,D,F	Ritchie et al. (1987)
Wheat	mech		mech	mech	mech	mech	mech	mech	I,W,T,D	Stapper (1984)
Wheat	mech		mech		mech	mech	mech	mech	I,T,D	Weir et al. (1984)
Maize	emp		mech	mech	mech	mech	mech	mech	I,W,T,D	Stapper and Arkin (1980)
Rice	mech	mech	mech	mech	mech	mech	mech	mech	I,W,T,D,F	Ritchie et al. (1986)
Maize	mech	mech	mech	mech	mech	mech	mech	mech	I,W,T,D,F	Jones and Kiniry (1986)
Rice	emp	emp	emp	mech	emp	emp			I,W,T	Angus and Zandstra (1980)

Key to Submodels:
emp = empirical approach used.
mech = mechanistic approach used.

Key to Environmental Factors:
I = irradience; W = water status (rainfall, humidity, wind); T = temperature; F = fertilizer, nutrient status; D = day length.

Key to Processes Which May be Described in Submodels:
1 Phot = Light interception and photosynthesis; canopy architecture; radiation characteristics; leaf characteristics.
2 Nutr = Root activity and nutrient uptake: root system architecture; soil nutrient status; root status and characteristics.
3 Part = Partitioning: substrate pools of carbon compounds and nutrients replenished by 1 and 2; transport between pools; utilization of pool substances for growth; priorities.
4 Transp = Transpiration: water balance of plant and soil; water status of plant.
5 Gr & R = Growth of structural dry matter and the recycling of structural components; respiration.
6 LA exp = Leaf area expansion.
7 Dev = Development and morphogenesis: initiation, growth and development of new organs (stems, leaves, flowers, fruits, storage organs, etc.)
8 Sen = Senescence.

Source: Modified after France and Thornley (1984) and Legg (1981).

nitrogen dynamics. The simulation of nutritional effects on crop growth requires a crop growth model which has several key components where the effects of nutrition could interact. The processes which would be required in this general model for a nitrogen submodel to be attached are described below.

2.3.1 Interface Between Crop Growth Models and N Dynamics Models

The rates of most of the soil nitrogen transformation processes are dependent on soil moisture availability. Denitrification occurs during periods of excess water in the profile and nitrate leaching is associated with water movement in the profile. Mobility of the nitrate and ammonium ions which plants take up is highly dependent on soil water content (Nye and Tinker, 1979). Thus to adequately simulate nitrogen dynamics and their consequences for crop growth and yield, a soil water balance component which describes water movement and water content is a necessity.

Nutrient uptake has been shown to be a function of nutrient concentration, moisture content, root length density and plant demand (Nye and Tinker, 1979). For prediction of nutrient uptake, some knowledge of the changes in root distribution through time is required. Some uptake models require these data as specific inputs (e.g., Claassen and Barber, 1976). Since these root length density data are only rarely available, a model which can predict them is required to add a nutrient model. In some instances (e.g., Davidson, 1978a) an assumed distribution of roots through the profile is used to facilitate uptake calculations. This ignores any dynamic effects of nutrient supply and environment on root growth. Since the growth of roots in

soils is very variable, simulating root distribution provides one of the greatest challenges to crop modellers although separate models for this (Lungley, 1973; Porter et al., 1986) could possibly be adapted for this purpose.

Nutrient stresses and environmental stresses affect many crop growth processes which ultimately determine the rate of biomass production and the formation of crop yield. Some of the crop growth processes known to be affected by nutrition are:

1. Leaf area development (Biscoe and Willington, 1984).
2. Photosynthesis per unit leaf area (Hunt, 1984).
3. Shoot/root partitioning (France and Thornley, 1984).
4. Tillering (Masle, 1984).
5. Rate of grain filling (Vos, 1984).
6. Crop ontogeny (Biscoe and Willington, 1984).

To adequately simulate the effects of N deficiency on crop growth, appropriate description of these processes and the provision of "attach points" needs to be made. The most common approach to this has been to ascribe a scalar index to nitrogen status to reduce the rate of a particular process from some potential. Angus and Zandstra (1980) achieved this in their rice model by devising a nitrogen index (NI) based on the crop nitrogen status. This index was multiplied by several environmental indices to determine a growth index and ultimately crop growth.

2.4. Nitrogen Dynamics Models

Many different simulation models exist which describe some or all of the N-cycle processes occurring in cropping systems. Some of

these were the subject of the proceedings of a workshop (Frissell and van Veen, 1981) and of excellent reviews by Tanji (1982) and Myers (1986). Several of the models cited in these reviews are concerned with specific aspects of the N cycle such as ammonia volatilization (Parton et al., 1981), leaching (Addiscott, 1981; Burns, 1980) and denitrification (Smith, 1981; Leffelaar, 1981). Most of the models are primarily concerned with the major soil processes in the N cycle and few consider the N dynamics of a growing crop. Several very comprehensive models containing details linking together all the major soil transformations have also been developed. Amongst them those of van Veen (1977) and Molina et al. (1983) provide considerable detail about the functioning of the various transformations at the microbiological level.

Other models have been developed with the specific purpose of examining aspects of pollution from organic wastes and from excessive fertilization, (e.g., Rao et al., 1981; Selim and Iskandar, 1978, 1981; and Donigian and Crawford, 1976). Some models such as those of Watts and Hanks (1978), Tillotson et al. (1980) and Tanji et al. (1981) simulate most of the major soil transformations of nitrogen as well as the uptake by the crop, but fall short of fully describing the system in that the crop growth and yield response is not incorporated. PAPRAN (Seligman and van Keulen 1981), a simulation model which predicts dry matter production as limited by water and nitrogen, aims to do this for pastures in semiarid environments.

A table indicating the level at which various processes have been modelled, and input requirements and the type of computations used has been assembled (Table 2.3) for several nitrogen dynamics

Table 2.3. A Compilation of Simulation Models of Nitrogen Dynamics in Cropping Systems

Author	Primary Function of Model	MI	N	D	MB	L	AV	AE	U	CG	PNP	WB	Testing	Data Requirements	Time Step
Tanji et al. (1981) and Tanji (1982)	Water and nitrogen fluxes in irrigated maize	M	M	M	O	M	O	O	S	O	O	M	L	L	<1
Wagenet et al. (1977)	Monitoring transformation of urea fertilizer added to soil	O	M	M	O	M	S	E	E	O	O	M	L	M,L	<1
Rao et al. (1981)	Pollution model based on earlier work of Davidson et al (1982)	M	M	M	O	M	O	M	E	O	O	M	L	L	<1
Selim and Iskandar (1981)	Model for nitrogen behavior in soils receiving liquid wastes	O	M	M	O	M	O	M	M	O	O	M	L	L	<1
Hagin and Amberger (1974), and Kruh and Segall (1981)	Original model to examine N and P load added to drainage waters--later adapted to field crop	E	M	M,P	O	P,M	O	O	P	O	O	M	L	L	<1
van Veen and Frissel (1981) and van Veen (1977)	Model describing role of micro-organisms in N transformations	M	M	M	M	M	E,M	M	O	O	O	O	L	L	<1
McGill et al. (1980)	Very detailed model of C & N dynamics in grassland soils	M	M	M	M	E,S	O	O	E,M	O	S,O	O	O	L	<1
Seligman and van Keulen (1981)	Model for pasture growth in semi-arid regions	P	O	O	O	P	S	O	P	P	P	P	L	M	1
Parton et al. (1981)	Model simulates volatilization losses from urine patches	O	O	O	O	O	M	M	O	O	O	O	O	L	<1
Addiscott (1977)	Model primarily for leaching on structural soils but expanded to accommodate other trans-formations	E	E	O	O	P	O	E	O	O	O	P	L	M	1
Duffy et al. (1975)	Model designed to predict nitrate concentration in tile drain effluents	S	S	S	O	E,M	O	O	S	S	O	E	L	M,S	1
Burns (1974, 1975, 1976)	Model for prediction of leaching on sandy soils	O	O	O	O	P	O	O	O	O	O	P	L	M	1
Richter et al. (1980)	Simulation model to predict N availability on a specific soil type	E	O	O	O	E	O	O	O	O	O	E	L	M,L	1
Knapp et al. (1983)	Mineralization and microbial biomass model	M	O	O	M	O	O	O	O	O	O	O	L	L	<1

(Continued)

Table 2.3. A Compilation of Simulation Models of Nitrogen Dynamics in Cropping Systems (Continued)

Author	Primary Function of Model	MI	N	D	MB	L	AV	AE	U	CG	PNP	WB	Testing	Data Requirements	Time Step
Greenwood et al. (1974)	Dynamic model describing effects of soil and weather on N response in lettuce	O	O	O	O	E	O	O	M	E,M	E	O	L	M,S	1
Greenwood et al. (1984)	Simple model for describing relationships between supply of N and growth for sugar beets	S	O	O	O	E	O	O	M	E	E	O	L	S	1
Zartman et al. (1976)	Uptake model for tobacco	O	O	O	O	O	O	O	M	O	O	O	L	L	?
Scotter et al. (1984)	Simple site-specific model describing fate of urea	E	E	S	O	E	S	O	E	O	O	E,S	L	S	1?
Reddy et al. (1979a,b)	Model designed to examine impact of point-source pollution from animal wastes	E,S	S	O	O	O	E,S	O	O	O	O	O	-	S	?
Chen (1976)	An outline of model for use in large area simulation. No development to the stage of testable product is reported	E,S	E	E	O	O	O	O	E,S	S	S	O	O	?	?
Watts and Hanks (1978)	Model for water balance and N uptake in corn	E,S	O	O	O	M	O	O	P,M	O	O	M	L	M	<1
Tillotson et al. (1980) and Tillotson and Wagenet (1982)	Modification of earlier Wagenet model	O	M	M	O	M	S	M	E,M			M	L	L	<1
Davidson et al. (1978a,b)	Simulation of N dynamics in crop lands receiving wastes	M	M	M	O	M	O	M	M	O	O	M	L	L	<1
Molina et al. (1983)	Comprehensive simulation model examining tillage effects on nutrient dynamics	M	M	M	O	M	M	M	M	M	M	M	L	L	<1

Processes included as components in the models:
MI = Mineralization and/or immobilization of N.
N = Nitrification of ammonium.
D = Denitrification.
MB = Microbial biomass.
L = Movement of nitrate within the soil.
AV = Ammonia volatilization.
AE = Ammonium adsorption and exchange.
U = Uptake of nitrate and ammonium by the crop.
CG = Crop growth.
PNP = Partitioning of N within the plant to various organs.
WB = Soil water balance.

NOTE: For explanation of entries listed under processes, testing, and data requirements see text. The time step is indicated as being of less than 1 day or 1 day.

models. A brief description of the various alternative approaches to modelling each of the major nitrogen transformations is included in Chapter 3.

One notable feature of all the models tabulated in Table 2.3 is that none of them simulate all of the processes listed. Most of the models listed had been subjected to some testing but none had undergone extensive testing across a diversity of data sets. Most testing was confined to data sets used for the purposes of model development. In many cases the authors argued there were insufficient data generally available to adequately test their models (McGill et al., 1981; Selim and Iskandar, 1978). These statements are perhaps indicative of creation of models with data requirements far beyond those which it is realistic to expect to be available.

The table broadly indicates the level at which processes are modelled and is not intended to be definitive. The amount of input data required by the models and the degree to which they have been tested is similarly indicated. The approaches used to model the various processes differ widely and categorizing the methods used is difficult. In many cases several different levels of approach may have been adopted and there is arguably some overlap between the classifications used.

Some models utilize a mathematical approach based on kinetic theory and/or systems of solution of simultaneous differential equations. In the table these approaches are coded as "M". These models generally require the input of various rate constants and specific coefficients. These models are mechanistic and provide some statement as to how a particular process occurs in terms of the underlying mechanisms.

At the opposite level of complexity is a purely empirical approach which does not attempt to describe mechanisms underlying a particular process and in which the relationships used lack generality. Regression modelling approaches are generally in this category. Models in these cases are generally only reliable within the bounds of the data set used to generate them. These are coded with an "S" in the following table.

Intermediate to these approaches is a mechanistic approach which is sufficiently general to have widespread applicability and which has simple data requirements. Models of this type may depend upon "rational empiricisms" to describe various process. These models employ the phenomenological approach described previously. These are coded with a "P" in the table.

One further criterion on which models may be distinguished is the amount and type of input data required to run them. For a model to be useful to a diversity of users it should require only a minimum of commonly available data. A minimum data set for rice has been proposed (Angus and Zandstra, 1980) and more recently a workshop to define a minimum data set for use in "agrotechnology transfer" has been held (Kumble, 1984). A more specific definition of this minimum data set including data collection procedures has been proposed by Jones (1984). The minimum data set required by the CERES models (Godwin et al., 1984; Jones et al., 1984) follows these latter two definitions. The MDS comprises daily climatic data, some soils and plant data which are usually available from agricultural research stations. In Table 2.3 models which require data substantially beyond the MDS are coded with an "L" and those with data requirements

similar to the MDS are coded with an "M". Those models which require substantially fewer data are coded with an "S".

From an analysis of Table 2.3 it would appear that no model exists which can adequately describe the major factors influencing supply of N to the crop, its subsequent uptake and utilization and the determination of crop yield and yet depend only on an MDS for input. To satisfy the needs of a diversity of potential users a model which achieves these ends and utilizes only a minimum data set and which is readily verifiable is needed. The CERES-WHEAT-N model described in the following chapter is designed to meet these goals.

2.4.1 Comparison of Models

Five of the models listed in Table 2.3 were independently tested for their ability to simulate soil mineral N availability over time by de Willigen and Neeteson (1985). For the study, data were collected from a field experiment in the central Netherlands. Over a 7-month period soil samples were taken fortnightly to a depth of 90 cm and analysed for moisture and mineral N. Data describing the soil physical properties, crop residues, and soil organic matter as well as the necessary meteorological data were assembled for each of the models. Comparisons were made between measured soil mineral N and that simulated by each model (Table 2.4). A sixth model (Zandt and de Willigen, 1981) which had previously been calibrated against these data was also compared.

Table 2.4. A Comparison of Six Soil N Dynamics Simulation Models

Regression coefficients of the line yzax + b, where y = measured nitrate contents of the upper 60 cm, and x = simulated nitrate contents of upper 60 cm.

Model	a	b	r
Addiscott (1977)	0.92 ± 0.05	11.9 ± 2.5	0.99
Burns (1974)	1.05 ± 0.24	1.53 ± 11.3	0.84
Seligman and van Keulen (1981)	0.67 ± 0.86	52.4 ± 4.0	0.94
Richter et al. (1980)	0.86 ± 0.47	14.9 ± 16.5	0.68
van Veen and Frissel (1981)	1.21 ± 0.21	25.0 ± 9.9	0.90
Zandt and de Willigen (1981)	1.03 ± 0.16	8.20 ± 7.3	0.92

(Adapted from de Willigen and Neeteson (1985).

Performance was judged by calculating a regression line for each model with the simulation results for the upper 60 cm as the dependent variable and the corresponding observed data forming the independent variable. In this analysis the regression coefficients "a" and "b" should ideally have zero and unity values, respectively. While there is some danger in drawing too many conclusions from performance compared to one data set, it is noteworthy that the two models constructed from very simple functions and requiring only a minimum of data performed best. De Willigen and Neeteson (1985) indicated that subsequent testing of the Zandt and de Willigen model on a different data set indicated poor performance. The models of Seligman and van Keulen (1981) and Richter et al. (1980) both tended to overestimate N mineralization. The most detailed model, that of van Veen and Frissel (1981), performed most poorly.

The testing indicated that in many cases a similar answer could be achieved by different methods. If this proves to be true across a diversity of data sets, then in the interests of efficiency the simplest method and the one requiring the fewest data inputs should be chosen. The method chosen, however, must still contain sufficient detail to accommodate phenomena which may be important in other data sets. A real challenge for modellers then is not only to describe how a particular process operates but also to define the appropriate level for modelling the process.

2.5. Statement of Model Requirements and Conclusions

As a tool to facilitate N fertilizer research for wheat grown in rainfed and irrigated areas, a comprehensive model is required which can:

1. Describe the growth and yield response to additions of N fertilizer in diverse wheat growing environments.
2. Identify causes of inefficiency of fertilizer N utilization and where possible define the magnitude of losses of N from the system.

An appropriately designed operational model could be used in the following applications:

- Assistance with farm planning.
- Risk analysis for strategic planning.
- Within-year management decisions.
- Large area yield forecasting.
- Policy analysis.
- Agro-climatic zoning.

- Identification of fertilizer responsive area.
- Definition of research needs.

Ritchie and Otter (1985), cognizant of the limitations encountered in making a model useful for a specific purpose, have defined the main features needed for a user-oriented model which would achieve these objectives:

1. The input information on weather, soils, and genetics should be available.
2. It should be written in a familiar computer language.
3. The computational time should be a minimum.

To broaden the audience of possible users of such a model, compatibility with the personal computer environment and compatibility with the minimum data set can be added.

From the review above it is apparent that some of the crop models have some but not all of the features required to meet this prescription. Most of the crop-oriented models have shortcomings in descriptions of the soil transformations of N as well as being unable to account for differences between crop cultivars. Conversely, most of the soil-oriented models, while providing extensive description of the soil processes, fail to describe the crop component. Clearly a model which has balance between these two approaches and meets the goals defined above is needed. The CERES-WHEAT-N model described in the following chapter incorporates most of the features above. It is an attempt to provide a user-oriented globally applicable model of wheat growth and yield as affected by climate, variety, soil types, and nitrogen status.

Table of Contents

3.1. Overview

The CERES WHEAT model is a user oriented simulation model of wheat crop growth, development and response to nitrogen. It is designed to be able to simulate wheat growth and response to N in any environment where wheat is grown given the appropriate data. Its structure is sufficiently flexible for the model to be useful in the many applications listed previously. To enable application to these diverse problems, a model design constraint has been to limit input data requirements to only those which could reasonably be attained from field experiment stations.

The original version of the model had no nitrogen component and was thus designed to simulate crops in situations where nitrogen was not limiting. This version of the model described the effects of weather, soil physical properties, and genotype on crop growth, development and yield. The model was not designed to simulate the effects of other factors which may reduce yields such as weeds, pests and diseases, and other nutrients. These effects are not included in the model since the factors are more random in nature and can usually be controlled through management practices. Simulation of these components would have been inordinately difficult and would have added further complexity to the model. Components which simulate the major nitrogen transformations were added and appropriate interfaces to the water balance, growth and development routines of the main model were made. The non-nitrogen components of the model have been described by Ritchie and Otter (1985). A brief description of some of these components is made in the following section where it contributes to the understanding of the nitrogen components. This chapter describes the nitrogen component of the

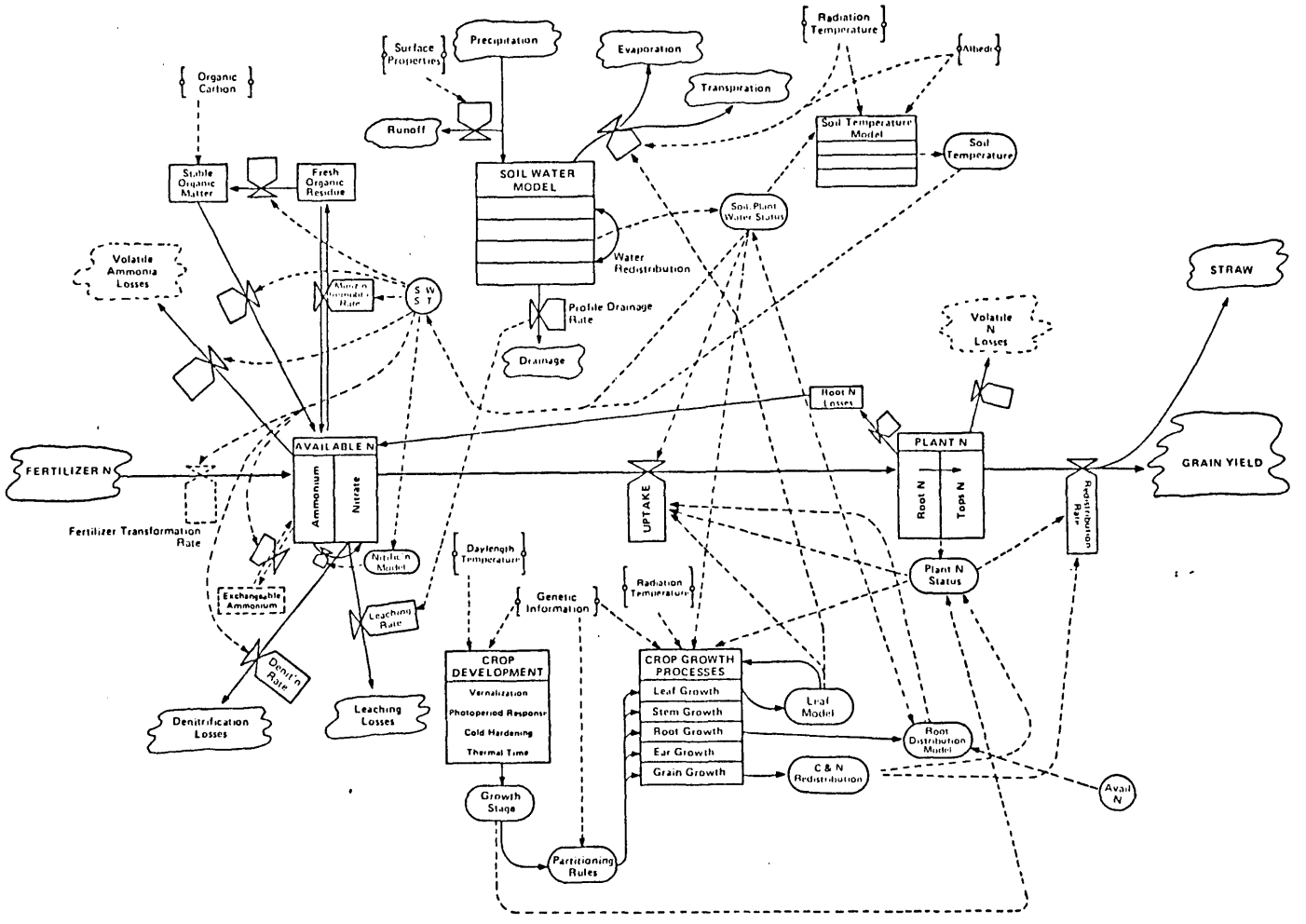

Figure 3.1. Systems Diagram of the CERES-WHEAT Model: Solid Lines = Material Flows; Dotted Lines = Information Flows; Dotted Lines Enclose Items Not Described. SW = Soil Water, and ST = Soil Temperature.

model and examines various approaches to modelling each of the major processes.

The CERES WHEAT model simulates evapotranspiration, soil water balance, crop ontogenetic development, and the growth of leaves, stems, ears and roots. The nitrogen component of the model adds to this the description of the movement of nitrate, mineralization and immobilization of N associated with the turnover of organic matter in the soil, nitrification, denitrification, and the uptake of N and its utilization by the crop. The various interrelationships and feedbacks among the processes modelled are illustrated in Figure 3.1. An important objective during model development has been to strive for a state of balance by not incorporating more detail about certain processes while ignoring or oversimplifying other equally important processes.

The model utilizes a daily time step and is designed to be relatively computationally efficient and yet maintain code which is sufficiently explicit for most users to follow. It is written in the language FORTRAN-77 and will run on a diversity of computers with only trivial modification. The computer time required to simulate one complete growing season from seeding to harvest varies according to the length of the growing season, the number of soil layers simulated and the amount of output required. Typical average values vary from 2 to 3 seconds for a large mainframe computer (e.g., AMDAHL 470/V8) to about 5 minutes on an IBM personal computer.

The model consists of a series of subroutines with a separate subroutine for each major process. The names and functions of each of these subroutines and the interlinkages between them are indicated

on the following flowcharts (Figures 3.2 a,b,c,d,e). A listing of the model, a glossary of the variables used and a sample output are appended (Appendices 1, 2, 3). A standardized system for model inputs and outputs for the CERES WHEAT model, the CERES MAIZE model (Jones and Kiniry, 1986) and the SOYGRO soybean model (Wilkerson et al., 1983), has been devised (IBSNAT, 1986). This system enables these models and others under development to share a common data set, which should facilitate modelling studies where multiple crops are being simulated. The input system enables interactive selection of crop genotypic, weather, soils and management data appropriate to the experiment being simulated. Figure 3.2a flowcharts this selection process. The structure and format of all required model inputs is described in IBSNAT Technical Report 5 which is appended (Appendix 3).

After selection of the appropriate inputs, the model initializes the necessary variables for growth, water balance, and soil nitrogen dynamics simulation, and displays these parameters for checking before commencing simulation. These initializations are accomplished in the subroutines depicted in Figure 3.2b. The model uses two switches which are provided as input parameters. One of these (ISWNIT) enables the model to be run with the assumption that N is nonlimiting and thus none of the N transformation calculations are calculated. The second switch (ISWSWB) enables the model to be run with the assumption that water is nonlimiting and thus water balance calculations are not performed. These options can reduce input requirements substantially and decrease execution time markedly. Following initializations a daily simulation loop is entered in which

one day's weather data is read and then all calculations on water and N balance, crop growth and development are performed (Figures 3.2c,d). A series of switches is used to route execution to different subroutines dependent upon the stage of crop development and whether the soil profile is draining. After these calculations are completed output may be written to the output files (Figure 3.2e). The simulation continues by returning control to the point of reading the next day's weather data.

3.2. Water Balance

The model incorporates a soil water balance component which includes calculation of surface runoff, drainage, evaporation from the soil surface, upward flow of water, and plant-water extraction. The soil water balance model operates on a layer-by-layer basis with the layer depths and storage characteristics as input parameters. Two field determined limits of plant available water are employed in the simulation; a lower limit (LL(L)) (volume fraction) and a drained upper limit (DUL(L)). Procedures exist (Ratliff et al., 1983) for determining appropriate values for these parameters from commonly available soil parameters. Soil water in each layer typically varies between these limits but may become temporarily wetter than DUL(L) after rainfall or irrigation and before drainage is complete. The field saturated water content SAT(L) is employed in the drainage calculations. SAT(L) is the maximum water content possible in a layer.

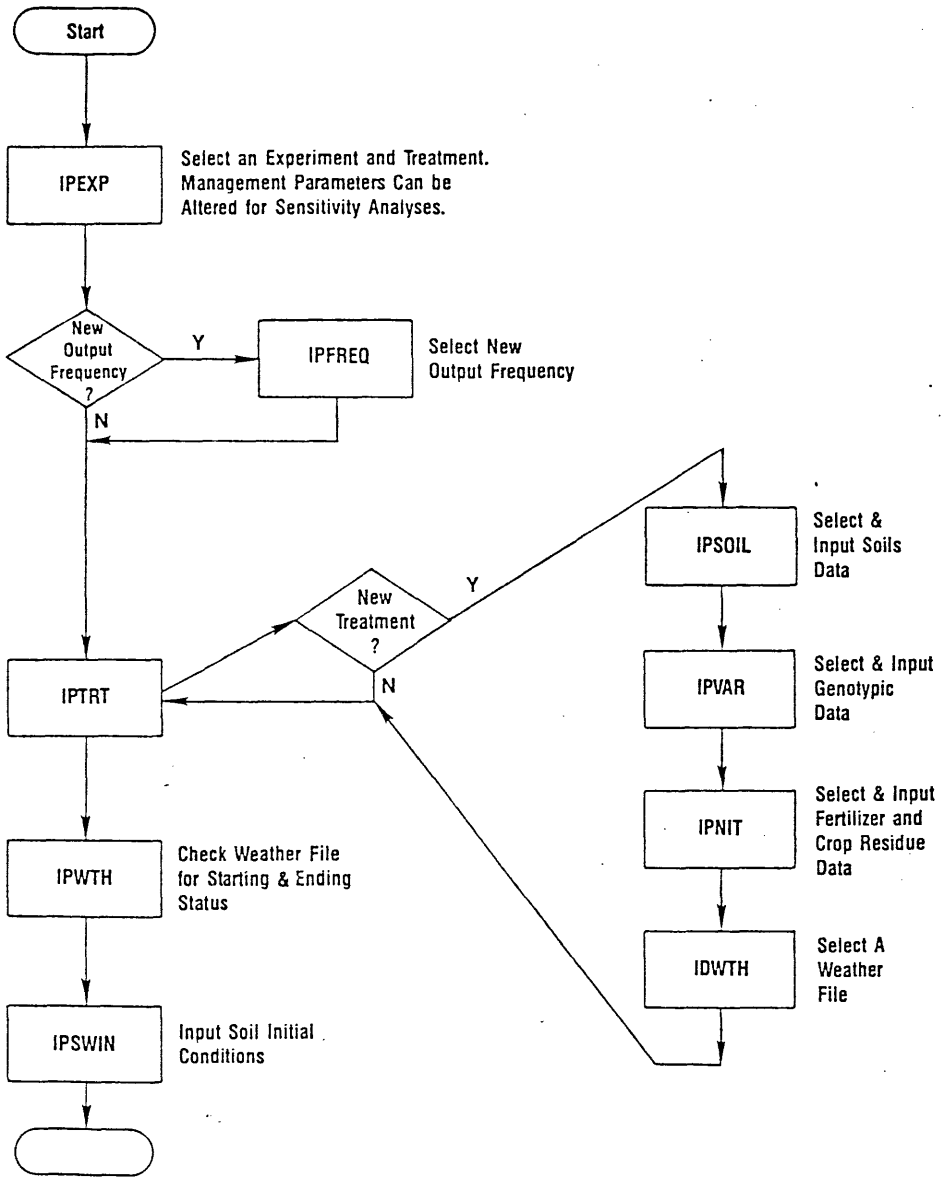

Figure 3.2a. Input Selection Routines.

Figure 3.2. Flowchart for the CERES-WHEAT Simulation Model Subroutine Names are Indicated in the Rectangular Boxes. In a Normal Simulation Control Passes From the Routines Depicted in Part (a) to (b), (c), (d), and (e) and During the Cropping Season is Returned to (c). When the Crop is Mature Control Returns to Part (a).

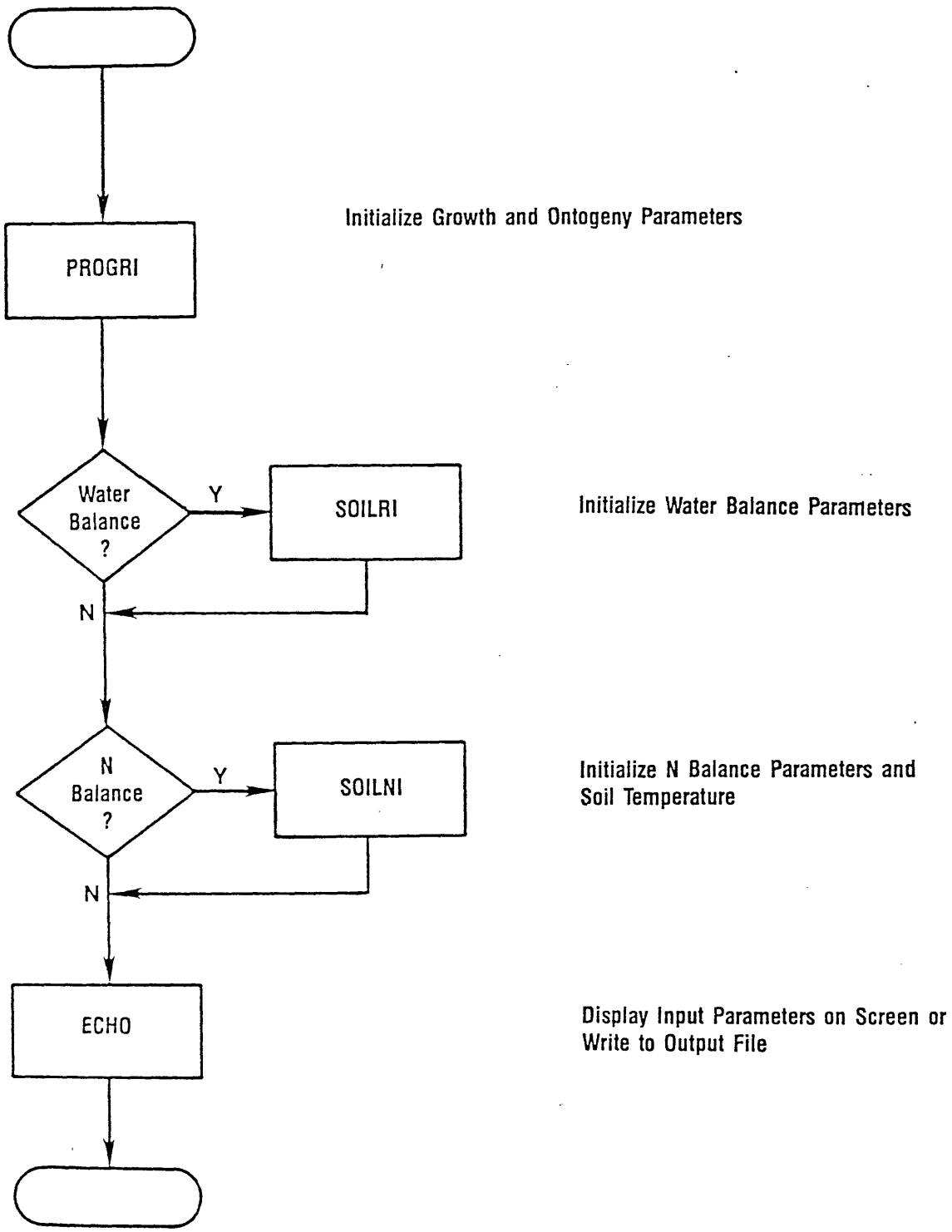

Figure 3.2b. Initialization Routines.

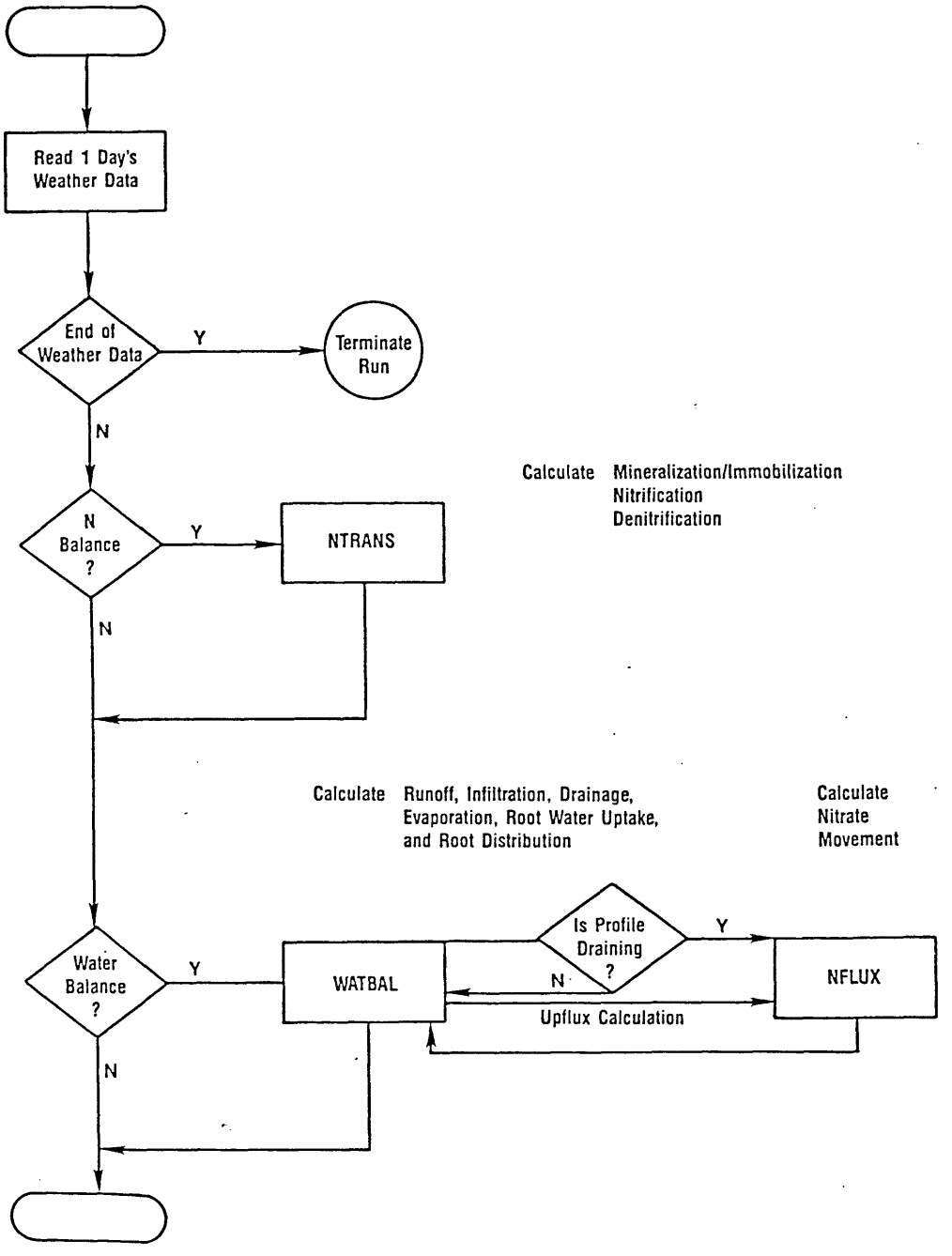

Figure 3.2c. Subroutines for Nitrogen Transformations, Water Balance, and Leaching.

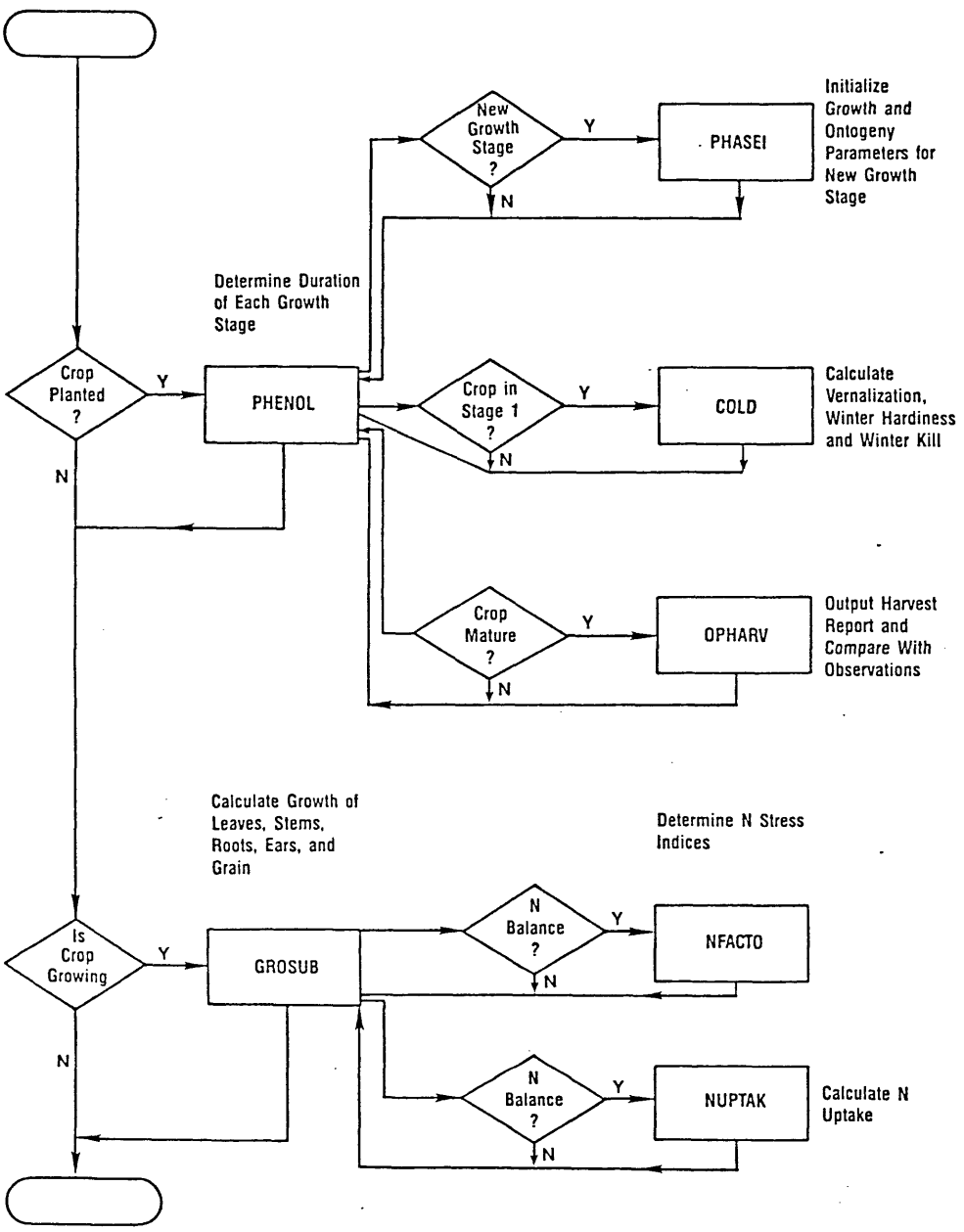

Figure 3.2d. Subroutines for Crop Growth, Phasic Development, Response to Cold Temperature, Response to Nitrogen, and N Uptake.

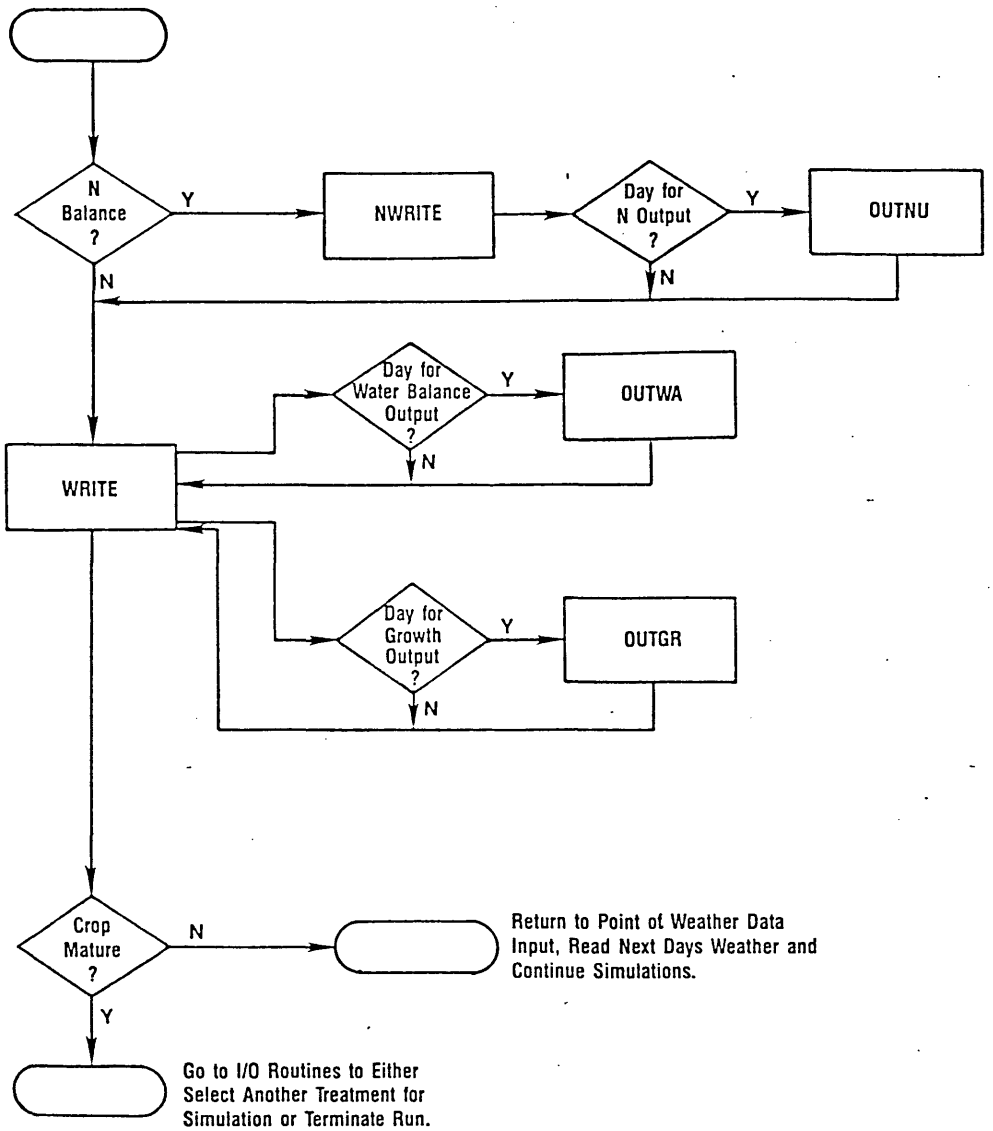

Figure 3.2e. Output Subroutines.

Other water balance related inputs required by the model are the soil albedo (SALB), the upper limit of stage 1 evaporation (Ritchie, 1972) (U), a constant for calculating the profile unsaturated drainage rate (SWCON) and the curve number used to calculate runoff (CN2). The water balance model has been described by Ritchie (1984). These inputs together with the values for initial soil water present in each layer at the commencement of simulation are read in the input/ output component of the model.

The subroutine SOILRI provides for initialization of the evaporation and runoff routines. The daily calculations of water balance are performed in subroutine WATBAL. This routine firstly adds any irrigations which may have occurred on a day to precipitation which may have occurred on that day. It then determines the amount of this total which ran off using a modification of the USDA-Soil Conservation Service (SCS) curve number method (Williams et al., 1983). Remaining water is assumed to have infiltrated (PINF), and the resulting redistribution of water in the soil profile and drainage out of the root zone is calculated using the approach flowcharted below (Figure 3.3). The volumes of water moving by unsaturated flow (DRAIN) and that moving by saturated flow (the excess of PINF over HOLD) are summed for each layer and preserved in an array (FLOW(L)) which is later utilized in the nitrate flux calculations.

Following drainage, the water balance model calculates evapotranspiration. Upward flow of water in the top four soil layers is calculated following subtraction of the soil evaporation (ES) from the upper layer. Capability exists for the water to also move in a downward direction if conditions are appropriate. The values for

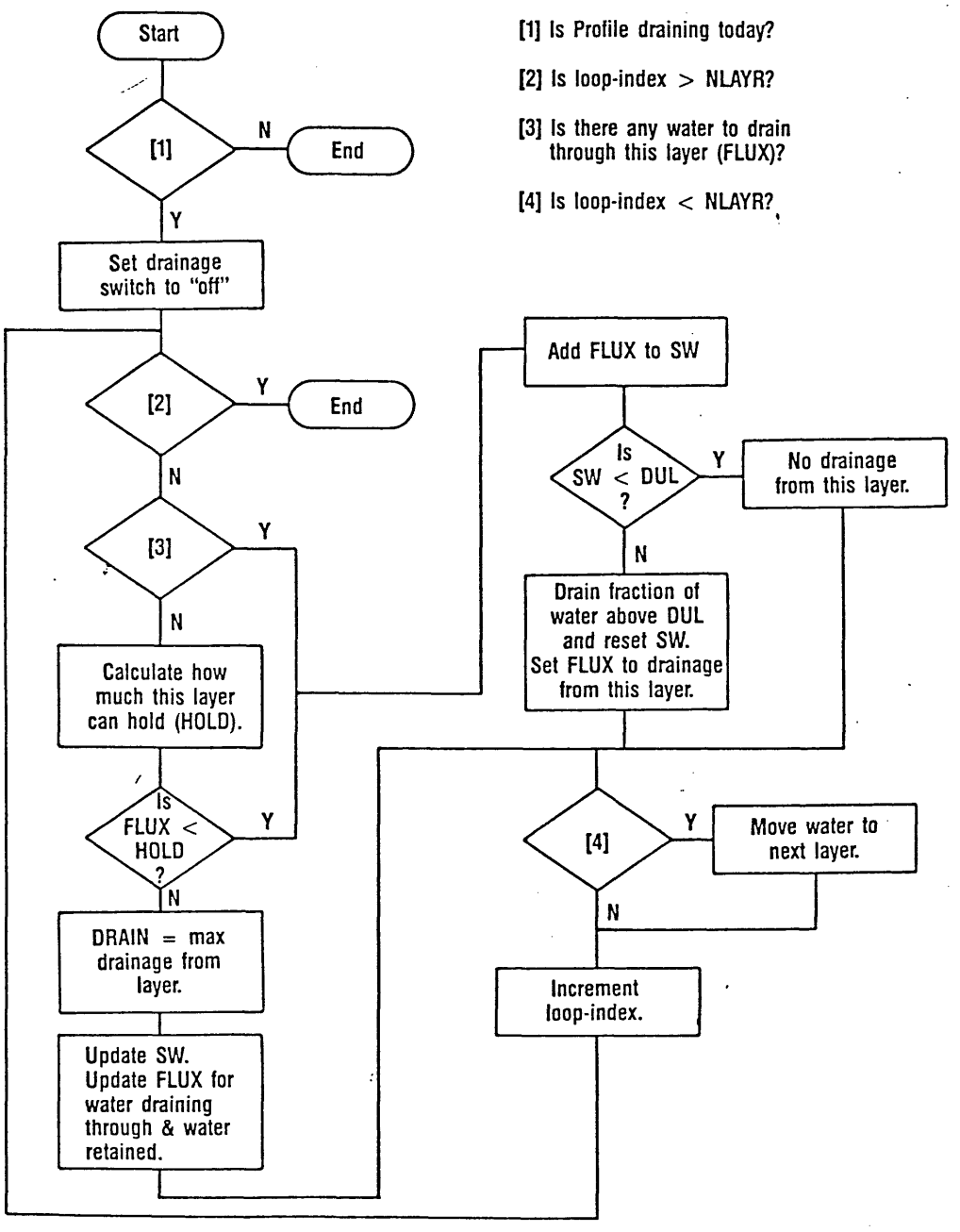

Figure 3.3. Flowchart of the Drainage Component of the Water Balance Subroutine (WATBAL) in the CERES-WHEAT Model. Key:
FLUX = Volume of Water Moving Into a Layer.
HOLD = Volume of Water a Layer Can Hold Up to Point of Saturation.
SW = Volumetric Moisture Content.
DUL = Drained Upper Limit of Moisture Content.
NLAYR = Number of Layers in Profile.

flow of water from each layer are preserved in the array (FLUX(L)) for later use in the nitrate flux calculations.

Root-water uptake from each layer is then calculated and the balance adjusted. Two soil water deficit factors, SWDF1 and SWDF2, are also determined in this subroutine. They have values between zero and unity and are calculated from the ratio of potential transpiration to potential root water uptake. These indices are used in the growth component of the model as described in a later section.

3.3. Nitrate Flux

Leaching of nitrate is probably the most common and the best understood N loss process. Nitrates leaching from soil often become a source of contamination of ground water, which has generated more recent interest in leaching from an environmental standpoint. The information available on leaching has been summarized in comprehensive reviews by Wild and Cameron (1980) and Nielsen et. al. (1982).

There have been many approaches to modelling leaching. Some of these have been based on multiple regression equations. Terry and McCants (1970) developed a regression model with variables describing the quantity of percolated water, soil porosity, CEC and various water-holding indices. The model was tested for various soils in column studies and worked well, but was not tested in the field. Other approaches have evolved around the use of more mathematically oriented mechanistic models (e.g., Childs and Hanks, 1977) and others have used a simple layering scheme (e.g., Terkletoub and Babcock, 1971) to describe water and solute flow. Addiscott and Wagenet (1985) have categorized simulation models for leaching into those

based on "rate" parameters and those based on "capacity" parameters (Table 3.1). The rate models for solute transport combine the description of several transport processes. Firstly water movement is defined in terms of the hydraulic conductivity and a potential gradient. This usually involves equations derived from Darcy's Law for water flow. Solute movement is then described in terms of mass flow and diffusion-dispersion. These models require inputs defining the soil hydraulic conductivity, the water potential gradient, and the apparent diffusion coefficient of the ion in the soil. It is often difficult to obtain meaningful values for many of these parameters from field experiments since they are subject to large degrees of spatial variability (Biggar and Nielsen, 1976). These mechanistic models have been used however, in some of the comprehensive nitrogen models listed previously (Table 2.3). It has been used in the pollution models of Selim and Iskandar (1981) and Rae et al., (1981) and in the models of N flux and transformation (Tillotson and Wagenet, 1982; and Wagenet et al., 1972) and in the tillage model of Molina et al., (1983).

Table 3.1. A Classification of Deterministic Leaching Models

A. Mechanistic (usually based on rate parameters)
   1. Analytical[a] (e.g., Neilsen & Biggar, 1962; van Genuchten & Wierenga, 1976)
   2. Numerical[a] (e.g., Childs & Hanks, 1977; Robbins et al., 1980)

B. Functional (usually based on capacity parameters)
   1. Partially analytical (e.g., De Smedt & Wierenga, 1978; Rose et al., 1982a,b)
   2. Layer and other simple approaches (e.g., Bresler, 1967; Tanji et al., 1972; Burns, 1974; Addiscott, 1977, Terkletoub and Babcock, 1971)

---

a. Refers to the solution of the flow equations.

(Adapted from Addiscott and Wagenet, 1985).

The number and nature of the inputs required by these models, and the manner in which they must be solved, renders them inappropriate for use in a management level model such as CERES. This had led to the development of simpler models based on capacity parameters. Capacity models define change (rather than rates of change) in amounts of solute and water content and are driven by amounts of water input. The simplest of these approaches is to assume the soil can be partitioned into layers and to calculate a discrete volume of water moving from one layer to the next in a cascading system. These simple approaches are no less reliable or less accurate in their simulations of water and solute movement than the more mechanistic models described previously (Addiscott and Wagenet, 1985).

Cameron and Wild (1982) compared three of the models listed in Table 3.1. Two of these, those of Burns (1974) and Addiscott (1977), are of this last mentioned category, and the third model of Rose et. al. (1982a,b) is more analytical in nature than these simpler models yet is driven by volumetric water inputs. The Burns model calculates solute movement from a layer according to the following function:

$$F = \left[\frac{P}{P + FC} \right] h$$

where:

F = fraction of solute moving from a layer.

P = amount of percolation from the layer (cm).

FC = moisture content of layer at field capacity (volume fraction).

h = depth of layer.

The model assumes instantaneous mixing of solute between water which is retained in the profile and water which is draining. In the Addiscott (1977) model, each layer is divided into mobile and retained phases on the basis of the soil moisture characteristic with the division between the phases at two bars. With infiltration, solute moves out of the mobile phase with piston flow. No equilibration with solute in the retained phase occurs until water movement has ceased. A later version of the model (Addiscott, 1981) allows for solute diffusion between the phases rather than the instantaneous equilibrium after water movement has stopped. This separation of solute between mobile and retained phases is of more importance on structured soils. This point of separation between mobile and retained water, however, will probably vary among soils as will the rate of equilibration between pools. The Rose et al., model proved most successful for Cameron and Wild (1972) in predicting chloride movement on a soil derived from chalk when irrigated or with rainfall. Minor modification, however, to both the Burns (1974) and Addiscott (1977) models greatly improved their performance. This modification was to pass water through the profile in 5-mm increments rather than as a single parcel. While the Rose et. al. (1982a,b) model yielded the best fit to the observations, the model requires a field determined measure of dispersivity which is not commonly available. Addiscott and Wagenet (1985) concluded that these simpler, less mechanistic functional models are more appropriate to a management level model and they have modest data inputs which are usually obtainable. Their reliance on capacity type soil water inputs enables them to avoid the spatial variability problems associated with the rate inputs.

In the CERES models nitrate N may move between layers in the profile but the movement of ammonium is not considered. Nitrate flux calculations are performed in subroutine NFLUX.

Nitrate movement in the soil profile is highly dependent upon water movement. The volume of water present in each layer (SW(L) * DLAYR(L)) and the water draining from each layer ((FLUX(L)) in the profile is used to calculate the nitrate lost from each layer (NOUT) as follows:

NOUT = SNO3(L) * FLUX(L)/(SW(L) * DLAYR(L) + FLUX(L))

A fraction of the mass of nitrate (SNO3(L)) present in each layer thus moves with each drainage event.

A simple cascading approach is used where the nitrate lost from one layer is added to the layer below. When the concentration of nitrate in a layer falls to 1.0 μg NO_3 per g of soil then no further leaching from that layer is deemed to occur. The method used may be termed a "reservoir mixing model" and is similar to the approach used by Burns (1974), but water movement is controlled by the SWCON variable in the drainage routine. The implicit assumption is that all the nitrate present in a layer is uniformly and instantaneously in solution in all of the water in the layer. Thus no attempt is made to separate nitrate in solution between the retained water and the mobile water. Differences in the relative volumes of retained water and mobile water between clays and sands occur as a function of the relative magnitudes of LL(L), DUL(L), and SAT(L). The rate of nitrate flux is also sensitive to changes in SWCON since this variable determines the rate of drainage.

Nitrate is more readily displaced from sands since the volume of water which can move ((SAT(L) - DUL(L)) * DLAYR(L)) is large in comparison to the retained water (DUL(L) * DLAYR(L)). Most of the difference in simulated leaching rate between soils of different texture is explained by this difference in proportion of water which is mobile. Some difference is also attributable to the rate at which profile can drain (SWCON).

The upward flow of water in the top four soil layers will also cause some redistribution of nitrate. A second loop commencing in the deepest layer of evaporative water loss (MU) is used to calculate this redistribution. Nitrate moving from a layer (NUP) is calculated as a function of upward water movement (FLOW(L)) in a manner identical to leaching:

NUP = SNO3(L) * FLOW(L)/(SW(L) * DLAYR(L) + FLOW(L))

No upwards loss from the top layer occurs by this process.

Since there will occasionally be instances when this slowly moving water can move in a downward direction (negative values of FLOW(L)) a third loop starting in the top layer and running to the fourth layer is also used. These instances would occur when a small rainfall wets the top layer of a very dry profile. There may have been insufficient water for drainage to occur but a moisture potential exists between the top layer and the second layer initiating this flow. The resultant movement of nitrate will be very small.

3.4. Soil Nitrogen Transformations

The CERES model simulates the decay of organic matter and the subsequent mineralization and/or immobilization of N, the nitrification

of ammonium and denitrification in subroutine NTRANS. Fertilizer addition and transformations (assumed to be instantaneous) are also performed in this subroutine.

3.4.1. Fertilizer Additions

Fertilizer N is partitioned in the model between nitrate and ammonium pools according to the nature of the fertilizer used. Fertilizer products are specified by a numeric code IFTYPE and can be urea (1 or default 0), ammonium nitrate (2), any ammoniacal source such as ammonium sulphate, ammonium phosphate or anhydrous ammonia (3), calcium ammonium nitrate (4), any nitrate source such as potassium or sodium nitrate (5). The model assumes instantaneous hydrolysis of urea and thus its behaviour is simulated identically to that of ammonium. A preliminary urea hydrolysis procedure is described in Chapter 8. As well as the numeric code for fertilizer type, inputs required to describe the fertilizer are: the date of application (JFDAY), the amount of N applied (AFERT) and the depth of placement (DFERT). For any placement depth the assumption is made that the fertilizer is uniformly incorporated into the layer. Layer thicknesses are supplied as input and are usually based on natural horizonation in the profile. Surface fertilizer applications are treated as being uniformly incorporated into the top layer. Up to 10 split applications can be accommodated by the model.

3.4.2. Mineralization and Immobilization

N mineralization is defined as the transformation of N from the organic state into the inorganic forms of NH_4^+ or NH_3 (Jansson and Persson, 1982). N immobilization is defined as the transformation of inorganic N compounds into the organic state (Jansson and Persson, 1982). Both processes are closely linked to the microbiological turnover of organic matter which usually contains more than 95% of the soil's nitrogen (Vlek et al., 1983). Immobilization occurs when soil microorganisms assimilate inorganic N compounds and utilize them in the synthesis of the organic constituents of their cells. A balance exists between the two processes. When crop residues with a high C:N ratio are added to soil, the balance can shift resulting in net immobilization for a period of time. After some of the soil carbon has been consumed by respiration net mineralization may resume. N mineralized from the soil organic pool often constitutes a large part of the nitrogen available to the crop. Thus, predicting the precise N fertilizer needs of a crop requires an assessment of the nitrogen-supplying capacity of the soil (Stanford, 1982).

This requirement has led to the development of various laboratory procedures for estimating the N-supplying capacity of soils. Stanford and Smith (1972) developed an incubation procedure to estimate two parameters (N_0 and K) of a simple mineralization model. The model was of the form:

$$N = N_0 (1 - e^{-Kt})$$

where:

N = net N mineralized at time t.

N = potentially mineralizable N.

K = rate constant.

t = time (weeks).

Several refinements to the laboratory procedures to shorten the incubation time were made (Stanford and Smith, 1976; Stanford and Smith, 1978), leading to a technique based on an acid permanganate extraction to estimate N_0. In the field, soil water and temperature are major constraints to the rate of mineralization. To accommodate these effects, a temperature index (Stanford et al., 1973) and a water index (Stanford and Epstein, 1974) are used to scale the rate of mineralization to conditions prevailing in the field.

The simplicity of the model and its verification by Stanford and coworkers on a diversity of soils makes it attractive to adaptation into a form usable by a comprehensive model such as CERES. Inconsistencies in the mineralization rate predicted by this model on some soils, however, have led some workers (Molina et al., 1980; Jones, 1984) to propose two-pool models. These models have one pool of rapidly mineralizing N and one pool of a more slowly mineralizing N. Other workers (Smith et al., 1980; Talpaz et al., 1981) have maintained the single pool model but adjusted the functional form. The requirement for laboratory procedures to estimate N_0 and K limits the application of the model. Jones et al. (1984) have attempted to overcome some of this limitation by using a regression procedure to estimate N_0 and K from other soil properties. The procedure was based on an analysis of Stanford's data of U.S. soils and some Chilean soils. The authors note the procedure should not be used on tropical soils since these were not included in the database. Some other soil types were only sparsely represented and the method would need some caution in its use.

The Stanford approach gives no consideration to soil carbon and is not suited to examining the effects of addition of crop residues of various types. To accommodate some of these difficulties more microbiologically oriented models have been developed. These models subdivide the soil organic N into several pools and simulate environmental effects on microbial biomass (McGill et al., 1981; Parnas, 1975; Smith, 1982; van Veen and Frissel, 1981; Knapp et al., 1983). These approaches provide insights into microbial dynamics and balance the flow of N with the flow of carbon. These models require many soil and site specific inputs, and often require the initialization of pools which cannot be measured (Myers, 1986). The overall complexity of these models and their data requirements have meant they have only rarely been tested outside the locations where they were developed. Among the more comprehensive models cited previously (Table 2.3) most have described mineralization and immobilization with first-order kinetics (e.g., Tanji et al., 1981; Rao et al., 1981; Selim and Iskandar, 1981). Rate constants need to be determined for each soil and site before these models can be run.

The perceived application for the CERES models in studies examining crop growth and fertilizer management requires that a mineralization model be simple, requires few inputs, and will work on a diversity of soils. Simulation studies examining the effects of crop residues also require that the model be capable of simulating the fate of residues of different compositions. Other studies examining the potential role of nitrification inhibitors (see Chapter 6) require a model wherein the processes of ammonification and nitrification are separated. The approach used in the CERES-WHEAT model is based on a

modified version of the mineralization and immobilization component of the PAPRAN model (Seligman and van Keulen, 1981). This model is an attempt at maintaining some of the functionality of the micro-biological level models but doing so at a very simplified level.

The modifications to the model have been to simulate nitrification rather than assume it to be an instantaneous process, and to partition the fresh organic matter pools simulated so that an interface to the denitrification procedures could be constructed. Modifications were also made to temperature and water indices to fit the CERES water balance and soil temperature routines. The mineralization and immobilization routine simulates the decay of two types of organic matter. Unless indicated otherwise the coefficients used for the mineralization/immobilization functions described below were drawn from the PAPRAN model. These are fresh organic matter (FOM) which comprises crop residues or green manure and a stable organic or humic pool (HUM). Three pools comprise the FOM pool in each layer (L), vis:

FPOOL(L,1) = carbohydrate

FPOOL(L,2) = cellulose

FPOOL(L,3) = lignin.

In PAPRAN, FOM is simulated as one pool and the decay rate constant selected according to the proportion of the initial amount of FOM remaining. In CERES separation of FOM into three pools enabled a better estimate of soluble carbon which is used in the denitrification routine.

These three pools are initialized as a fraction of the FOM(L) pool in subroutine SOILNI. Initially, the FOM(L) contains 20% carbohydrate, 70% cellulose and 10% lignin. The model requires as input data the amount of straw added, its C:N ratio and its depth of incorporation (if any). An estimate of the amount of root residue from the previous crop is also required. This can be crudely estimated as being 20% of the previous season's crop yield (this assumes a 50% harvest index and a root:shoot ratio at harvest of 0.1). A default value of 500 kg/ha is assumed if no data are available. Based upon these data, initial values of FOM and the N contained within it (FON) for each layer are calculated in subroutine SOILNI. A further input required by the mineralization routine is the soil organic carbon in each layer (OC(L)). This is used to calculate HUM(L) and, together with a simplifying assumption of a bulk soil C:N ratio of 10, is used to estimate the N associated with this fraction (NHUM(L)).

Each of the three FOM pools (FPOOL (L,1 to 3)) has a different decay rate (RDECR (1 to 3)). Under nonlimiting conditions the decay constants as reported by Seligman and van Keulen (1981) are 0.80, 0.05, and 0.0095 for each carbohydrate, cellulose, and lignin, respectively. The decay constant for carbohydrate implies that under nonlimiting conditions 80% of the pool will decay in one day. Nonlimiting conditions very seldom occur in soils since one or all of soil temperature, soil moisture, or residue composition will limit the decay process. To quantify these limits three zero to unity dimensionless factors are calculated.

A water factor (MF) is first determined from the volumetric soil water content (SW(L)) relative to the lower limit (LL), drained upper limit (DUL) and saturation (SAT). When the soil is drier than DUL, MF is calculated as:

AD = LL(L)*0.5

MF = (SW(L)-AD)/(DUL(L)-AD)

where,

AD = air dry moisture content (volume fraction).

When the soil is wetter than DUL, MF is calculated as:

MF = 1.0-(SW(L)-DUL(L))/(SAT(L)-DUL(L))*0.5.

The functions follow the observations reported by Myers et al., (1982) and Linn and Doran (1984) of moisture effects on ammonification. The first function allows ammonification to proceed at slow rates when soil moisture content is below the lower limit of plant water availability. Reichmann et al., (1966) have reported ammonification occurring in soils drier than 1.5 mPa and this would approximately correspond to LL. Under very wet conditions (100% of water filled porosity), ammonification proceeds at approximately half of the rate of ammonification at field capacity (Linn and Doran, 1983). The comparative effects of soil moisture on the simulated rates of ammonification, nitrification and denitrification can be seen in Figure 3.4.

A temperature factor (TF) is calculated directly from soil temperature (ST(L))

TF = (ST(L)-5.0)/30.0.

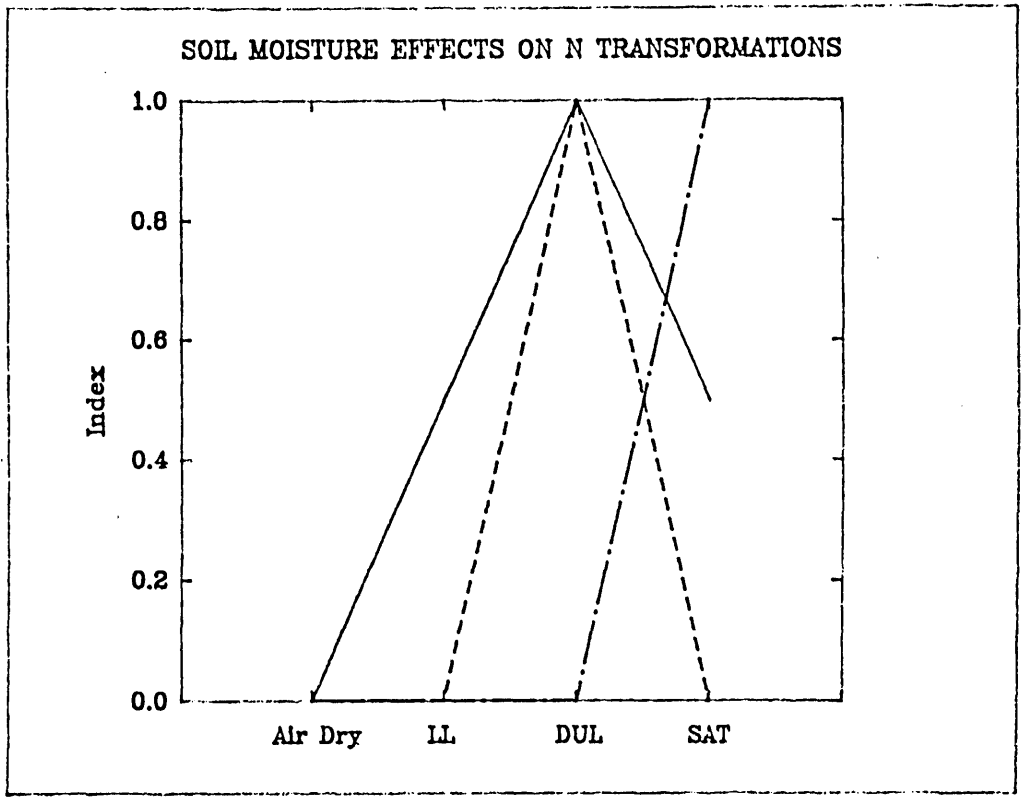

Figure 3.4. Effects of Soil Moisture on Nitrogen Transformation Rates.

LL = Lower Limit.
DUL = Drained Upper Limit.
SAT = Saturation Moisture Content.
——— = Ammonification.
- - - = Nitrification.
– · – = Denitrification.

This approximates the soil temperature effects on ammonification reported by others (Stanford et al., 1973; Myers, 1975). If the soil temperature (ST(L)) is less than 5°C then TF is set to zero and no decay occurs. The C:N ratio (CNR) imposes the third limit on decay rate. In this case C:N ratio is calculated as the C contained in FOM divided by the N "available" for the decay process. This N available for decay is the sum of the N contained in the FOM, which is FON, and the extractable mineral N present in the layer (TOTN). Thus,

```
CNR=(0.4*FOM(L))/(FON(L)+TOTN)
```

From CNR an index (CNRF) is calculated which has a critical C:N ratio of 25.

```
CNRF=EXP(-0.693*(CNR-25)/25.0)
```

When CNR is equal to 25, mineralization and immobilization are usually approximately in equilibrium (Harmsen and Kolenbrander, 1965; Russell, 1973). When CNR is less than 25, mineralization rate is not impeded by residue decomposition. In low N containing residues (e.g., freshly incorporated wheat straw) with a high C:N ratio, the N available for the decay process will greatly limit the decay rate (Figure 3.5).

For each of the FOM pools a decay rate (GRCOM) appropriate for that pool (JP) can be calculated.

```
G1=TF*MF*CNRF*RDECR(JP)
GRCOM = G1*FPOOL1(L,JP)
```

The gross mineralization of N associated with this decay (GRNOM) is then calculated according to the proportion of the pool which is decaying.

```
GRNOM = G1 * FPOOL(L,JP)/FOM(L) * FON(L)
```

GRCOM and GRNOM are summed for each of three pools in each layer.

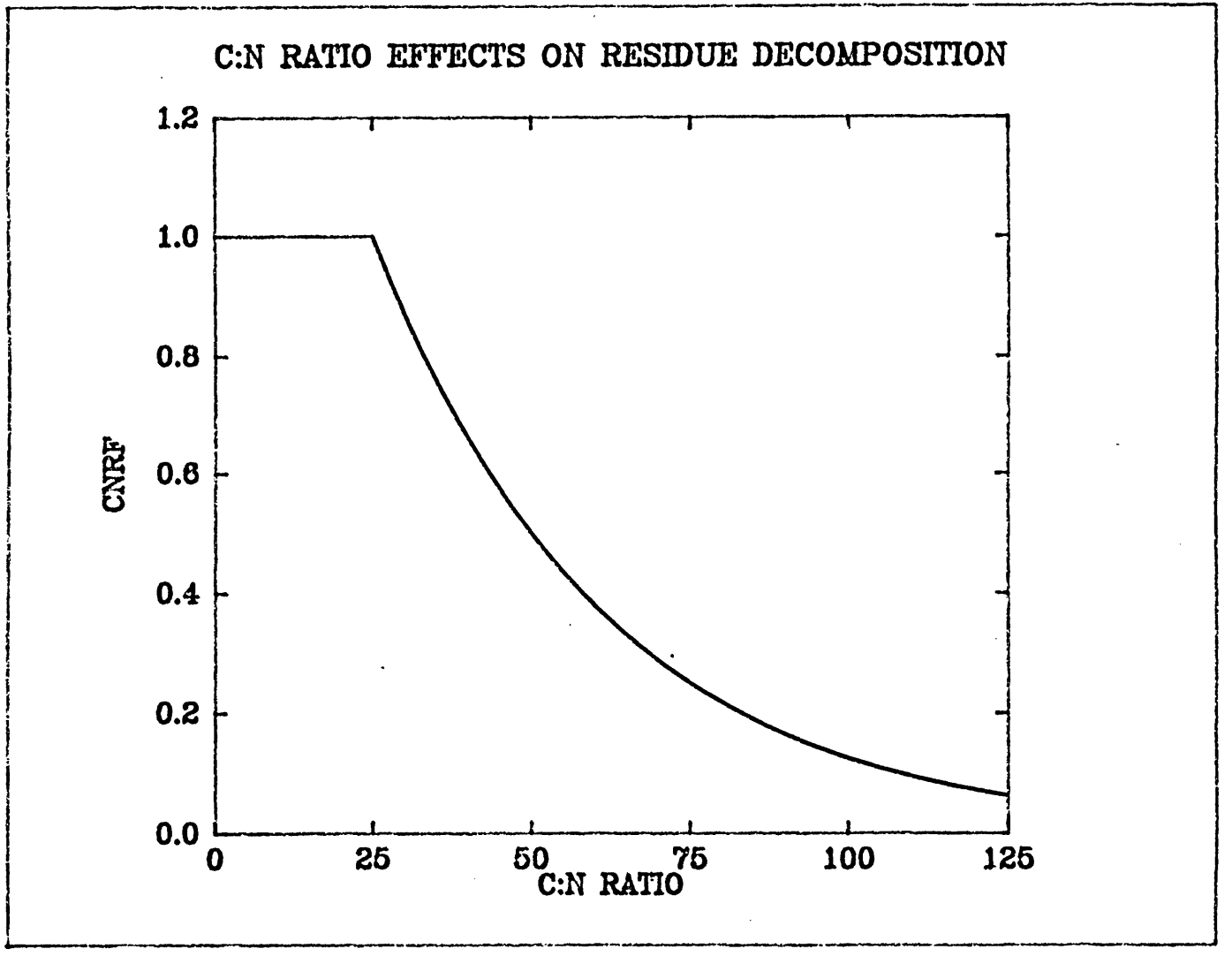

Figure 3.5. Effect of Carbon:Nitrogen Ratio on Residue Decomposition Rates.

The procedure used for calculating the N released from the humus (RHMIN) also utilizes TF and MF. In this case CNRF is not used and the potential decay rate constant (DMINR) is very small (8.3E-05). A further index (DMOD) was added to the RHMIN calculations to adjust the mineralization rate for certain atypical soils. On soils with chemically protected organic matter a less than unity value of DMOD is required so that mineralization is not overestimated. On freshly cultivated virgin soils a slightly greater than unity value has been found necessary to account for the sudden increase in mineralization activity. In all other circumstances a value of 1.0 is used for DMOD. Satisfactory alternatives for estimating DMOD are currently being sought. The procedure for calculating RHMIN then, is the product of the various indices and the N contained within the humus (NHUM(L)).

```
RHMIN=NHUM(L)*DMINR*TF*MF*DMOD
```

After calculating the gross mineralization rate, HUM(L) and NHUM(L) are updated.

```
HUM(L)=HUM(L)-RHMIN*10.0+0.2*GRNOM/0.04
NHUM(L)=NHUM(L)-RHMIN+0.2*GRNOM
```

These calculations also allow for the transfer of 20% of the gross amount of N released by mineralization of FON(L) (0.2*GRNOM) to be incorporated into NHUM(L)). This accounts for N incorporated into microbial biomass and has a concentration of 4% (0.04) determined as 0.1 g N/g C (soil C:N ratio of 10) multiplied by 0.4 g C/g OM (40% of OM is C).

As organic matter decomposes some N is required by the decay process and may be incorporated into microbial biomass. The N which is immobilized in this way (RNAC) is calculated as the minimum of the soil extractable mineral N (TOTN) and the demand for N by the decaying FOM(L).

RNAC=AMIN1(TOTN,GRNOM*(0.02-FON(L)/FOM(L))

where 0.02 is the N requirement for microbial decay of a unit of FOM(I). The value of 0.02 is the product of the fraction of C in the FOM(L) (40%), the biological efficiency of C turnover by the microbes (40%) and the N:C ratio of the microbes (0.125). FOM(L) and FON(L) are then updated (Seligman and van Keulen, 1981).

FOM(L)=FOM(L)-GRCOM

FON(L)=FON(L)+RNAC-GRNOM

The balance between RNAC and GRNOM determines whether net mineralization or immobilization occurs. The net N released from all organic sources (NNOM) is:

NNOM=0.8*GRNOM+RHMIN-RNAC.

Note that only 80% of GRNOM enters this pool since the remaining 20% was incorporated into NHUM(L). NNOM can then be used to update the ammonium pool (SNH4(L)).

SNH4(L)=SNH4(L)+NNOM

If net immobilization occurs (NNOM negative) ammonium is first immobilized, and if there is not sufficient to retain this pool with a concentration of 1 ppm, then withdrawals are made from the nitrate pool.

3.4.3. Nitrification

Nitrification refers to the process of oxidation of ammonium to nitrate. It is a biological process and occurs under aerobic conditions.

The main features which limit nitrification are: substrate NH_4^+, oxygen, soil pH, temperature, and carbon dioxide (see Focht and Verstraete, 1977, and Schmidt, 1982, for reviews).

There have been several different approaches to modelling nitrification. Van Veen (1977), van Veen and Frissel (1981), and McGill et al. (1980) modelled environmental effects on the populations of nitrifying bacteria and then calculated a nitrification rate based on this population. McGill et al. describe nitrification as a single-step process and van Veen and Frissel describe it as a two-step process. Both models require initial values of nitrifier populations as inputs and both operate with short time steps. These approaches are able to accommodate short-term lags in nitrification which may occur when nitrifier populations have been depleted.

Most models ignore microbial population aspects and describe nitrification as a simple first order kinetic process (e.g., Davidson et. al., 1978a,b; Tillotson et. al., 1980) with ammonium concentration as rate limiting variable. Tanji et. al. (1981), however, used a zero order kinetic function to describe nitrification. Most of the models described in Table 2.3 which utilize coupled differential equations to simulate the various N transformations require soil specific experimentally determined rate constants for nitrification as inputs.

The approach used in the CERES models has been to calculate a potential nitrification rate and a series of zero to unity environmental indices to reduce this rate. This potential nitrification rate is a Michaelis-Menten kinetic function dependent only on ammonium concentration

and is thus independent of soil type. A further index, termed a "nitrification capacity" index, is introduced which is designed to introduce a lag effect on nitrification if conditions in the immediate past (last 2 days) have been unfavorable for nitrification. Actual nitrification capacity is calculated by reducing the potential rate by the most limiting of the environmental indices and the capacity index. The capacity index is an arbitrary term introduced to accommodate an apparent lag in nitrification observed in some data sets. The functions updated below were found to be appropriate across the range of data sets tested.

The nitrification routine in subroutine NTRANS calculates the nitrification of ammonium in each layer. Firstly, an ammonium concentration factor (SANC) is calculated.

```
SANC=1.0-EXP(-0.01363*SNH4(L))
```

This is a zero to unity index which has approximately zero values when there is less than 1 ppm of ammonium present and has a value of 0.75 at 100 ppm.

The temperature factor calculated above for mineralization (TF) and a soil water factor for nitrification (WFD) (Figure 3.4) are used together with SANC to determine an environmental limit on nitrification capacity (ELNC).

```
ELNC=AMIN1(TF,WFD,SANC)
```

The water factor has a zero value for moisture content below the lower limit and increases linearly from the lower limit to the drained upper limit. Justine and Smith (1962) reported that nitrification did not occur below a water potential of 1.5 mPa. This function thus uses LL as a cutoff point for nitrification. To accommodate lags

which occur in nitrifier populations, ELNC and the previous day's relative microbial nitrification potential in the layer (CNI(L)) are used to calculate the interim variable RP2 which represents the relative nitrification potential for the day.

```
RP2=CNI(L)*EXP(2.302*ELNC)
```

RP2 is constrained between 0.01 and 1.0.

Today's value of the nitrification potential (CNI(L)) is then set equal to RP2. Since EXP(2.302*ELNC) varies from 1.0 to 10.0 when ELNC varies from 0.0 to 1.0, relative nitrification potential can increase rapidly, up to tenfold per day. An interim variable A is then determined from these indices and a zero to unity effect of soil pH on nitrification. This pH index is calculated in subroutine SOILNI and is similar to the function reported by Myers (1974).

```
A=AMIN1(RP2,WFD,TF,PHN(L))
```

This interim variable A is used together with the ammonium concentration (NH(L)) in a Michaelis-Menten function described by McLaren (1970) to estimate the rate of nitrification. The function has been modified to estimate the proportion of the pool of ammonium (SNH4(L)) which is nitrified on a day.

```
B=(A*40.0*NH4(L)/(NH4(L)+90.0))*SNH4(L)
```

A check is made to ensure some ammonium is retained in the layer and thus the daily rate of nitrification (RNTRF) is

```
RNTRF=AMIN1(B,SNH4(L))
```

Following this calculation soil nitrate and ammonium pools can be updated.

```
SNH4(L)=SNH4(L)-RNTRF
SNO3(L)=SNO3(L)+RNTRF
```

Finally, the soil temperature, moisture and NH4 after nitrification are used to update (CNI(L), which is used in the subsequent day's calculations.

```
SARNC=1.0-EXP(-0.1363*SNH4(L))
XW=AMAX1(WF,WFY(L))
XT=AMAX1(TF,TFY(L))
CNI(L)=CNI(L)*AMIN1(XW,XT,SARNC)
```

SARNC is a zero to unity factor for ammonium availability. WFD and WFY(L) are today's and yesterday's soil water factors, respectively, and TF and TFY(L) are today's and yesterday's soil temperature factors, respectively. The least limiting of the current day's and the previous day's water and temperature factors are used in the calculation of the new value of CNI(L). This prevents a single day of low soil temperature or water from severely reducing CNI(L).

It is important to note that the relative nitrification potential CNI(L) is calculated twice each day. Since (EXP(2.302*ELNC)) varies from 1.0 to 10.0, CNI(L) increases prior to the calculation of the nitrification rate. After nitrification, when the level of ammonium has declined, CNI(L) is reduced. The relative magnitudes of (EXP(2.302*ELNC) and AMIN1(XW,XT,SARNC)) determine whether relative nitrification potential increases or decreases over the short term.

3.3.4. Denitrification

Denitrification is the dissimilatory reduction of nitrate (or nitrite) to gaseous products including NO, N_2O, and N_2 (Knowles, 1981). Numerous methods have been developed to measure denitrification losses from soils. Quantitative estimates of N loss from agricultural

soils through denitrification vary tremendously from 0% to 70% of applied fertilizer N (Firestone, 1982). It is, however, difficult to measure directly these gaseous products of denitrification against the large background of atmospheric N. Because of this, the most frequently used method of determining losses has been to develop an ^{15}N balance and attribute the ^{15}N loss to denitrification (Hauck, 1979). This approach only describes total losses and does not distinguish among losses due to leaching, ammonia volatilization or denitrification. Thus in many instances denitrification has been overestimated and there are other situations where underestimation could also occur. Some progress on direct measures has been made (Bremner and Hauck, 1982; Tiedje et al., 1984; Craswell et al., 1985) which may provide more reliable estimates in the future. These difficulties in technique and the associated problems of data interpretation have greatly hampered the development and validation of universally applicable denitrification models.

Denitrification is a microbial process which occurs under anaerobic conditions and is influenced by organic carbon content, soil aeration, temperature and soil pH (see Focht and Verstraete, 1977, and Firestone, 1982, for reviews). Approaches to modelling denitrification have been many and varied. Much of the effort has concentrated on describing the aeration status of the soil and the onset of anaerobiosis as a predisposing condition for denitrification. Some models (Leffelaar 1979, 1981) describe water flux and oxygen diffusion from inter-aggregate spaces into aggregates. Others (Smith, 1981) add to this the diffusion of denitrification gases toward the atmosphere. McConnaughey and Bouldin (1985) have constructed a model which simulates the formation

of these anaerobic microsites and calculates the rate of denitrification as limited by the diffusion of solutes between aerobic and anaerobic zones. The effect of carbon availability and enzyme activity on denitrification rates were also included in the model. Microbial oxygen consumption as a function of microbial biomass, together with the processes determining oxygen movement in soils, is described in the denitrification sub-model of van Veen (1977). These approaches may be appropriate as research tools to study important parameters affecting denitrification on a micro-scale, but natural soil heterogeneity precludes their use on a broader scale. The small time-step and the requirement for inputs which are not commonly available also limit the applicability of these approaches.

Among the more comprehensive simulation models cited above (Table 2.3) denitrification is usually either ignored or simulated using simple kinetic functions. The models of Duffy et al. (1975) and Scotter et al. (1984) are exceptions to this and they use simplistic site specific empirical functions to describe the process. Most modellers describe the process as a first order process (e.g., McGill et al., 1981; Tanji et al., 1981; Davidson et al., 1981a,b) limited by nitrate concentration. Many of the models have also linked denitrification with the supply of carbon (e.g., Frissel and van Veen, 1981; Davidson, 1978a,b). In many instances an experimentally determined rate constant, specific for a given soil is required for the sub-model. Many of the models utilize very short time-steps. These would be inconsistent with the minimum data set and daily time step used by the CERES models.

The approach adopted in the CERES models has been to adapt the functions described by Rolston et al. (1980) to fit within the framework of the model and to match inputs derived from the water balance and mineralization components of CERES. The basic function used by these authors was also used by Davidson et al. (1978a) and was the subject of field testing under a variety of conditions in California. Predicted rates of denitrification compared favourably with direct measures of gaseous losses in the field experiments.

Denitrification calculations are only performed when the soil water content (SW) exceeds the drained upper limit (DUL). A zero to unity index (FW) (see Figure 3.4) for soil water in the range from DUL to saturation (SAT) is calculated.

```
FW = 1.0-(SAT(L)-SW(L))/(SAT(L)-DUL(L))
```

Linn and Doran (1984) used percentage of water filled porosity as an index of soil water availability effects on soil N transformations. Denitrification commenced with a water filled porosity of 60% and increased linearly up to 100% water filled porosity. This approximates the linear increase in FW as SW increases from DUL to SAT. (Similarly, Craswell (1978) reported a linear increase in the denitrification rate as soil moisture content was increased beyond that held at a tension of -10 mPa.)

A factor for soil temperature (FT) is also calculated.

```
FT=0.1*EXP(0.046*ST(L))
```

Rolston et al. (1980) using the data of Burford and Bremner (1976) and Reddy et al. (1979b) estimate the water-extractable C in soil organic matter (CW) as:

```
CW=24.5 + 0.0031*SOILC
```

In the CERES model SOILC is calculated as 58% of the stable humic fraction. To this is added the carbon contained in the carbohydrate fraction organic matter pool (40% of FPOOL(L,1)). Appropriate unit conversions are made using FAC(L) and the total water extractable carbon (CW) estimated.

```
CW = (SOILC*FAC(L)*0.0031+24.5+0.4*FPOOL(L,1)
```

Denitrification rate (DNRATE) is then calculated from the nitrate concentration and converted to a kg N/ha basis for the mass balance calculations.

```
DNRATE = 6.0*1.0E-05*CW*NO3(L)*FW*FT*DLAYR(L)
```

The interacting effects of soil temperature, soil water and additions of fresh organic matter can be seen in Figure 3.6. Following the calculation of DNRATE, the nitrate pool in the layer is updated with appropriate checks to ensure that a minimum concentration of nitrate is retained in the layer.

```
SNO3(L)=SNO3(L)-DNRATE
```

3.5. Soil Temperature

The soil temperature in each layer is used in the functions describing most of the major soil N transformations. The soil temperature model used in CERES is based on that used in the EPIC model (Williams et al., 1984). This method is based upon some simple empiricisms and requires only two inputs additional to those soil parameters required by the water balance and N transformation routines. These inputs are: TAV, the annual average ambient temperature and AMP, the annual amplitude in mean monthly temperature.

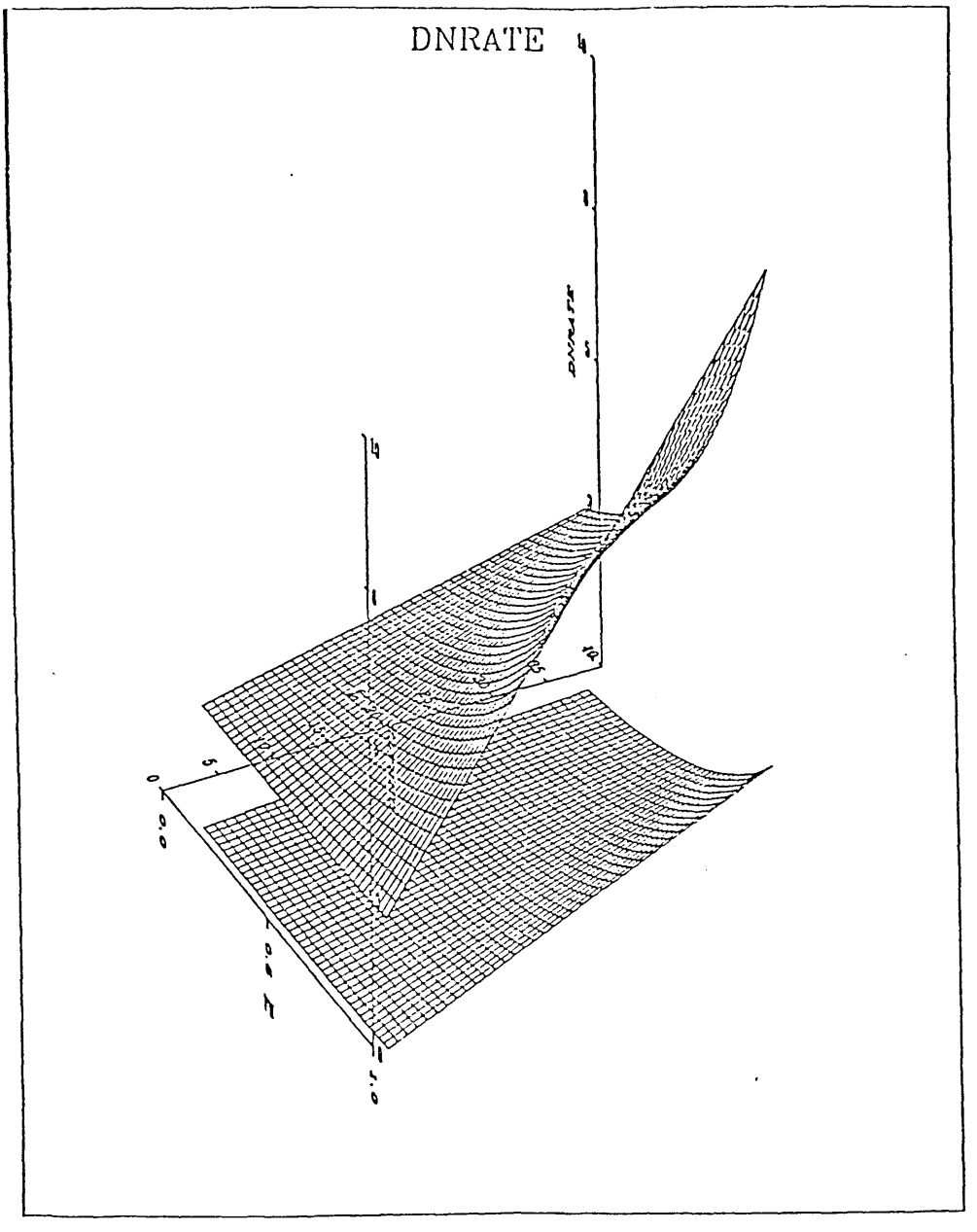

Figure 3.6. The Effect of Soil Temperature, Soil Water and Residue Addition on Predicted Denitrification Rate. The Upper Surface is for a Case Where 1,000 kg/ha of Carbohydrates Were Added to the Soil and the Lower Surface is for Case Where 200 kg/ha of Carbohydrate Were Added. The Vertical Axis Indicates the Simulated Denitrification Rate in kg NO_3 Lost/ha/day. The X axis (FW) Indicates Soil Moisture Over the Range From DUL (FW = 0) to SAT (FW = 1.0). The Y Axis (ST) Indicates Soil Temperature Over the Range 0° to 40°. The Simulations Were for a Soil Layer With Bulk Density = 1.3 g/cc, Organic Carbon = 1.5%, and Nitrate Concentrations of 30 ppm.

The method used to calculate the soil temperature at various depths in the profile requires the determination of a damping depth (the depth at which no diurnal variation in temperature is experienced). At depths shallower than this, diurnal change in temperature occurs with the greatest fluctuation occurring nearest the surface. The location of this damping depth (DD) is dependent upon parameters which influence the flux of heat in the soil, notably the bulk density and the moisture content. DD is updated daily to allow for changes in soil moisture content.

Soil surface temperatures are modelled as a function of the ambient temperature, the solar radiation, and the albedo. The 5-day moving average surface temperature is used to compute the temperatures in each layer as follows:

```
TMA(1) = (1.0-ALBEDO) * (TMN + (TEMPMX - TMN) * SQRT(SOLRAD/800.0)) +
     ALBEDO * TMA(1)
```

where:

TMA(1) = daily surface temperature

ALBEDO = the albedo of the soil surface and is an input variable for bare soils. As the crop canopy develops ALBEDO becomes a function of the leaf area. These calculations of albedo are performed in the water balance routine as they are a fundamental component of the evaporation model.

SOLRAD = solar radiation in langleys/day.

TEMPMX,TMN = daily maximum and mean temperature °C, respectively.

The long-term average daily ambient temperature (TA) for the current day of the year can be estimated from TAV and AMP.

```
TA = TAV + AMP * COS(ALX)/2.0
```

ALX is a variable (in units of radians) to relate the current day of the year (XI) to the time of the hottest day of the year (HDAY). In the northern hemisphere this is assumed to be day 200 and in the southern hemisphere day 20.

ALX = (XI - HDAY) * 0.0174

The coefficient 0.0174 is 1/365 days multiplied by 2π radians.

Deviations in the actual dates of the hottest day of the year in lower latitudes are of little importance since the volumes of AMP will be small and hence TA will approximate TAV.

The departure (DT) of the moving average temperature from TA is used in the calculation of the soil temperature in each layer (ST(L)) as follows:

ST(L) = TAV + (AMP/2.0 * COS(ALX + ZD) + DT * EXP(ZD)

where ZD = depth of layer L/current day's damping depth.

3.6. Phasic Development

Matching the phenology of the crop to the environment in which it grows is one of the most important aspects of matching crop requirements to environment. The CERES-Wheat model was developed to estimate the duration of the growth cycle of different wheat genotypes used throughout the world. The growth stages of wheat recognized by the model are organized around times in the plant's life cycle when changes occur in the partitioning of assimilate using the different plant organs. The changes in plant phenology occurring as the crop grows also influence the crop's requirement for N and its subsequent responses to N. At differing times in the plant's life cycle different parts of the plant are growing which have differing requirements for N

which must be accounted for separately. In CERES-Wheat the growth stages of the crop are numbered from 1 to 9 (see Table 3.2). This numerical coding system provides a convenient way of routing control through the major growth (GROSUB) and phenology (PHENOL and PHASEI) subroutines. Subroutine PHENOL is used to determine the duration of each phase and is called daily. Subroutine PHASEI initializes variables pertinent to a growth stage and is only called when growth stage changes.

Table 3.2. Growth Stages of Wheat as Defined in CERES-Wheat

Stage	Event	Plant Parts Growing	Factors Affecting Duration
7	Fallow or presowing	-	Management
8	Sowing to germination	-	Soil moisture
9	Germination to emergence	Roots, coleoptile	Seeding depth, temperature
1	Emergence to terminal spikelet initiation	Roots, leaves	Temperature, photosynthesis, vernalization
2	Terminal spikelet to end of leaf growth and beginning of ear growth	Roots, leaves, stems	Temperature
3	End of leaf growth and beginning of ear growth to end of pre-anthesis ear growth	Roots, leaves, ear	Temperature
4	End of pre-anthesis ear growth to beginning of grain filling	Roots, stems	Temperature
5	Grain filling	Roots, stems, grain	Temperature
6	End of grain filling to harvest	-	-

The inclusion of the variable (XSTAGE) is a modification of the original non-nitrogen version of the model. This was required to enable the calculation of plant critical N concentrations. These concentrations are determined as a function of crop ontogenetic age and are used within the model as part of the procedure to simulate the effects of N deficiency. The critical concentration functions (see Section 3.7) are based upon the often used Zadoks' growth scale (Zadoks et al., 1974). Zadoks' growth scale is a decimal index of crop development generalized for all cereals. The intervals between growth scale index values are based on crop morphological observations and are not related to a thermal time concept. To incorporate the Zadoks' scale, a scheme to provide a conversion between the integer growth stages recognized by the model (ISTAGE) and a functional form of the Zadoks' scale had to be devised. XSTAGE is used to determine an approximate value for the corresponding Zadoks' stage (ZSTAGE) with a series of functions (Table 3.3). The functions are located in subroutine NFACTO.

Table 3.3. Functions Used for Converting From Fractional Growth Stage (XSTAGE) to Zadoks' Growth Stage (ZSTAGE)

Morphological Stage	XSTAGE Range	Function
Emergence to terminal spikelet	0.0-2.0	ZSTAGE + XSTAGE
Terminal spikelet to booting	2.0-3.0	ZSTAGE = 2.0 + 2.0*(XSTAGE-2.0)
Booting to ear emergence	3.0-4.0	ZSTAGE = 4.0 + 1.7* (XSTAGE-3.0)
Ear emergence to anthesis	4.0-4.4	ZSTAGE = 5.7 + 0.8*(XSTAGE-4.0)
Anthesis to maturity	4.4-6.0	ZSTAGE = 6.02 + 1.86*(XSTAGE-4.4)

The daily maximum and minimum temperatures and a weighting procedure (Ritchie et al., 1987) are used in this subroutine to calculate a daily increment in thermal time (DTT). DTT is in units of day degrees, and is used as the primary factor affecting development rate. Other factors which affect the duration of each growth stage are indicated in Table 3.2.

During each model growth stage (ISTAGE), this thermal time is accumulated (SUMDTT) until sufficient thermal time has accumulated to necessitate a change of growth stage. When a new stage is encountered subroutine PHASEI is called and SUMDTT is reset to zero. Within each stage (ISTAGE) recognized by the model, a fractional stage (XSTAGE) can be calculated. Before each stage is entered the total thermal time required for the stage is fixed and thus the proportion of the stage which has passed on any given day may be estimated as:

SUMDTT/(Total thermal time required for stage)

XSTAGE is then calculated as ISTAGE plus this proportion. An exception to this scheme occurs in growth stage 1 where the thermal time for the duration of the stage is not fixed a priori but is also dependent on the combined effects of photoperiod and vernalization. The CERES model uses a system in which 400 development units are required to reach the end of stage 1. The rate of accumulation of these development units is dependent upon the cumulative amount of vernalization which has taken place, and the photoperiod and genetic coefficients specifying the sensitivity to these parameters. Thus fractional development can be estimated as the fraction of 400 development units which have passed.