**CERES Wheat 2.0**

**By**

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This is draft version of documentation for version 2 of the CERES wheat model. The sections dealing with running the model are now out-of-date and covered in DSSAT Users Guide. However much of discussion of the science in the model is still helpful. Some other more current articles are:

Ritchie, J.T.1991. Wheat phasic development. p. 31-54. In Hanks and Ritchie (ed.) [Modeling plant and soil systems. Agron. Monogr. 31](http://www.agronomy.org/spawn.cgi?target=mono/M_7&state=0887043847090), ASA, CSSSA, SSSA, Madison, WI.

Ritchie, J.T. and D.S. NeSmith. 1991. Temperature and Crop Development. p. 5-29. In Hanks and Ritchie (ed.) [Modeling plant and soil systems. Agron. Monogr. 31,](http://www.agronomy.org/spawn.cgi?target=mono/M_7&state=0887043847090)ASA, CSSSA, SSSA, Madison, WI.

Ritchie, J.T. 1998. Soil Water Balance and Plant Water Stress. p. 45-58. In Tsuji Y., Gordon Y. Tsuji, Gerrit Hoogenboom, Philip K. Thornton (Ed.)[Understanding Options for Agricultural Production](http://www.wkap.nl/book.htm/0-7923-4833-8). Kluwer Academic Publishers, Dordrecht. ISBN 0-7923-4833-8.

Ritchie, J.T., U. Singh, D.C. Godwin, W.T. Bowen. 1998. Soil Water Balance and Plant Water Stress. p. 83-102. In Tsuji Y., Gordon Y. Tsuji, Gerrit Hoogenboom, Philip K. Thornton (Ed.) [Understanding Options for Agricultural Production](http://www.wkap.nl/book.htm/0-7923-4833-8). Kluwer Academic Publishers, Dordrecht. ISBN 0-7923-4833-8.

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# CHAPTER 1

## INTRODUCTION

Simulation models of agricultural systems, when coupled with appropriate data sources, have a great potential for bringing agricultural research and development into the age of information technology. Within agricultural disciplines, crop production involves a complexity of interactions between crop genotype, the soil and aerial environment, and management practices. Considerable research has been done on the various components of crop production and some of their interactions. Much research has yet to be done. Some of the information has and is being used in models designed for specific uses such as crop growth, and some is being used more holistically to include broad aspects of agricultural systems.

This book documents a ten year collaborative project with the aim of producing a "user-oriented," general simulation model of wheat yields. The model was built to predict the performance of a particular cultivar, sown at any time, on any soil, in any climate. This goal may never be completely met due to the complexity of a biophysical system. However, even partially meeting the goal will provide considerable improvement in our ability to transfer agrotechnology information. Models help accomplish this goal by defining a minimum set of soil, weather, management, and genetic information that should be collected in practically all field experimental trials to help explain outcomes and thereby transfer the technology beyond the site and year of the trial. 

## HISTORY

This wheat modelling effort was started in 1977 when the USDA-Agricultural Research Service was asked to attempt an improvement in the U.S. government's capability to predict domestic and foreign wheat yields. Models prior to that time were mostly statistical, principally using monthly weather data. The CERES-Wheat model was one of three models initially developed by the USDA-ARS (Willis, 1985).

The belief that a crop model could be developed into a relatively simple user-oriented package came from the success of a model developed by one of us (Ritchie, 1972) to predict evaporation from plants and soils with incomplete cover. That model was more empirical than most models that were developed to predict evaporation and it has proven to work quite well under a wide range of conditions although it is not a mechanistic model. A feature that made it useful was the relatively few inputs required compared to a more mechanistic model. However, one constraint limiting the usefulness of the model was that the seasonal variations in leaf area index (LAI), information seldom available from experiments, was a necessary model input. To overcome this problem a model was developed to predict the LAI for a sorghum crop using principles of developmental physiology (Arkin, et al., 1976). LAI was found to be one of the most predictable quantities in crop modeling if the plant population and the leaf size distribution of a plant was known. Limitations of the sorghum model (SORGF) was that the number of leaves had to be input along with maximum leaf sizes because both the genotype and environment can affect leaf number and sizes. An initial goal of the CERES model was to predict leaf number and sizes by quantitatively describing how genetics and climate interact to determine the duration of vegetative growth in cereal crops. This information on LAI would provide the necessary information to more generally predict evaporation and light interception by plants.

The initial step in model development was to estimate duration and rate of crop growth as influenced by the aerial environment and the soil-water status. The next step was to link nitrogen dynamics to the system. The International Fertilizer Development Center was also interested in producing a model with this objective. As a result of that interest an agreement was made for IFDC to jointly develop the nitrogen dynamics routines as an addition to the model. D. C. Godwin was employed to work on that task in collaboration with J.T. Ritchie and C. A. Jones who then worked with the USDA-ARS in Temple, Texas. A nitrogen dynamics model for a maize model (CERES-Maize, Jones and Kiniry, 1986) and for the wheat model (Godwin, 1987) resulted from this effort. Also, to establish credibility for the model on a global scale, S. Otter-Nacke, a post-doctoral fellow from Germany began work on model testing using data sets from throughout the world. A detailed report on that testing effort has also been published (Otter-Nacke et al, 1987).

A multi-federal agency program called AGRISTARS was started in 1979 that provided funding to expand yield modeling. Consequently, Ritchie took on the leadership within USDA-ARS to develop a maize model in addition to the CERES-model. As a result of the AGRISTARS program, developing a user-oriented model for wheat and corn became a full-time objective of the Crop Systems Evaluation Research Unit at Temple, Texas until 1984. In 1984, Ritchie moved to Michigan State University. Since then, further model development and testing has been done there and at IFDC by Godwin.

Because of testing and improvement of the CERES-Wheat model since its beginning in 1977, several different versions of the model have been used for various purposes by several independent groups. Information they provided as feedback regarding model accuracy and user-friendliness, was helpful in improving the model. Two other models have been developed from early versions of the CERES-model as a result of specific interest in wheat modeling. A wheat model called TAMW, was developed by Mass & Arkin, 1980, as part of the Texas A&M University effort at Temple, Texas. The other model called SIMTAG, by Stopper (198xxx) was developed primarily for use in the dry areas in which the International Centre for Agricultural Research in Dry Areas (ICARDA) and the University of New England (Australia) were interested. Both models have much in common with the CERES-Wheat model.

In 1982 the International Benchmark Sites Network for Agrotechnology Transfer (IBSNAT), a USAID funded project at the University of Hawaii, decided to incorporate crop models into its program for international agrotechnology transfer. The CERES-Wheat and -Maize models were among those adopted by IBSNAT as a prototype system. The interest and financial support of IBSNAT has made possible the development of several other cereal crop models similar in detail to the CERES-Wheat and -Maize models. These crops include rice, sorghum, millet, and barley. Also, as a result of the IBSNAT Project, there has been a coordinated development of grain legume models for soybean (SOYGRO), peanut (PNUTGRO), and beans (BEANGRO) at the University of Florida. Present versions of the SOYGRO model (Wilkerson, et al. 1983), the PNUTGRO model (Boote et al., 1987),and BEANGRO have the same input requirements and level of detail as the CERES models thus giving users a wider variety of crop models to use with the same soil and weather input information.

To introduce crop models to a broad range of potential users, IBSNAT has held training workshops in Venezuela, Jordan, Taiwan, Malaysia, India, Bangladesh and Hawaii. These workshops have led several interested individuals to make significant suggestions regarding improvement of the model for technical and user friendliness purposes. In some instances, they have provided excellent data for model testing in various regions of the world.

Many of the ideas used in the model did not originate with the authors nor from technical literature. Several individuals other than those from our own institutions contributed time and expertise to the development of this model. Some collaborators for this project were transferred to Temple during the 1980-84 period by the Economic Research Service (ERS) and the Soil Conservation Service (SCS). Each agency had specific concerns that it wished to have represented in model development. The ERS was interested in resource economic policy questions and the SCS was interested in providing the necessary soil information for use of the model in regions where soil survey information was available. Scientists from the Foreign Agriculture Service, the National Oceanic and Atmospheric Administration (NOAA), and the National Aeronautical and Space Administration (NASA), have collaborated with us and contributed to the usefulness of the model.

At another level, a group of fellow researchers, to whom we are greatly indebted, provided unique contributions to the CERES-Wheat model. The original idea for quantifying the duration of growth stages of the crop as affected by weather and genotype came from H. A. Nix, CSIRO, Canberra, Australia, who provided continued encouragement and technical support throughout the project.

Dr. J. D. Hesketh, USDA-ARS, Urbana, Illinois, assisted with early experiments conducted at the Duke University Phytotron, and helped to quantify some of the concepts suggested by Nix. Tom Hodges and his colleagues at NOAA, in Columbia, Missouri, conducted tests of the model in foreign yield assessment and published a comparison of the phasic development predictions of CERES-Wheat with other models (Hodges, et al.,198xxx). Greg Larson, USDA-SRS, published the results of a sensitivity analysis of an earlier version of the CERES-Wheat model (Larson et al., 198xxx). The analysis provided feed-back for making several model improvements. 

## PURPOSE

The CERES-Wheat model was designed to simulate the effects of cultivar, planting density, weather, soil water, and nitrogen on crop growth, development, and yield. It was developed to be useful for prediction and control at the farm and regional level. These objectives partially dictated the level of detail of the model. The model is not principally intended to be an explanatory model for improving understanding of how the crop system works. The primary purpose is for predicting potential alternative management strategies and tactics that affect yield and intermediate steps in the yield formation process. It is also intended to be useful at the farm level for within year crop decision making and

multiyear analysis for risk assessment. On a regional basis it is intended to be useful for yield forecasting and the analysis of various policy questions related to crop production and resource conservation.

These purposes require that the model have the following characteristics:

o Use readily available weather, soil, and genetic inputs.

o Be written in a familiar and widely used computer language.

o Require minimal computation time.

o Be useful on microcomputers.

As a result of these constraints, most input data are available from or can be readily estimated from routinely collected daily weather data, standard soil characterization data, and data provided in the model documentation. The computer program is written in the familiar scientific language, FORTRAN.

To accurately simulate maize growth, development, and yield, the model takes into account the following processes:

o Phenological development, especially as it is affected by genetics and weather.

o Extension growth of leaves, stems, and roots.

o Biomass accumulation and partitioning, especially reproductive organs.

o Soil water balance and water use by the crop.

o Soil nitrogen transformations, uptake by the crop, and partitioning among plant parts.

A final purpose for the model is to identify knowledge gaps that can lead to improvements in the model's predictive capacity. Some of the gaps are highlighted in Chapter 9. 

## SYSTEM BOUNDARIES

To accomplish the primary purposes outlined above, it was necessary to exclude several potentially important factors that influence yield. The model focuses on how weather and genetic characteristics affect potential yield given a specified management scheme. Factors associated with management and weather however, are limited to plant-water supply and plant-nitrogen supply. We excluded phosphorous, potassium and other essential plant nutrients on the basis that they are often found in sufficient supply such that plant growth is not limited by them. Also, for the model to be more realistic, it should include linkages with pests and toxicities of various kinds. This model excludes those things as well as soil salinity and soil aeration problems. Catastrophic weather events such as hurricanes, hail storms or typhoons are not considered nor are yield reductions due to crop lodging. Many of these items could be incorporated into the model as a sub-routine if the need for that detail becomes warranted. Scientists from IFDC are planning a phosphorus linkage. Several pest management specialists are planning to link specific pest models with CERES-Wheat and other models adopted in the IBSNAT program. Published examples coupling pests to the IBSNAT crop models for predicting reduction in yield already exist (Berger and Jones, 1985; Boote, et al, 1983) although model tests have not yet been reported. 

## PHILOSOPHY REGARDING THE LEVEL OF DETAIL

The CERES-Wheat model was developed to include information from several scientific disciplines. To do this, maintaining balance in the entire model became our foremost principle. The predictions of the model can be no better than the level of detail of the least understood part of the model. It can not be made more accurate by including information from disciplines which are much better understood. Maintaining balance is somewhat similar to significant digits retained in mathematical functions. If a number with seven significant digits is multiplied by a number with two significant digits, the product is no better than the two significant digit number.

To maintain balance, it seemed clear to us that crop biomass growth needed to be calculated independently of the plant development. Biomass growth has been the focal point of many comprehensive crop models which have been developed to date. Our philosophy is that development and growth had to be treated in balance for the model to produce realistic predictions because each factor is affected by the environment and stresses in different ways.

Realistic model prediction also depends on accurate input information. Model inputs of soils and weather that are potentially spatially variable limit the ability to accurately predict the spatially variable area. The important inputs that usually are spatially variable include depth of effective rooting in the soil and rainfall amounts measured with a rain gauge that is often located some distance from the field. Variation in rooting depth is difficult to measure but influences the supply of water and nutrients for the plants. When water and nutrient supplies are marginal, spatial variability in plant size is often observed within fairly small areas of a field. This creates a degree of uncertainty in model predictions that must be considered when deciding on the level of detail to be used. 

## THE NEED FOR USER-ORIENTED MODELS

With declining profitability and natural resources becoming more scarce, farm managers and regional policy planners require new tools to assist in decision making. Simulation models that can capture the major edaphic and genetic effects on crop growth as well as the nuances of weather offer good opportunities for assisting farm managers in several aspects of decision making.

Farmers make decisions that are surrounded by natural and economic uncertainties, mainly weather and prices. Agricultural research is designed to provide information that will help the farmer in making such decisions. It is almost impossible, however, for research to provide specific answers, because field experiments cannot include all possible soil types and weather sequences.

Many farmers make decisions based on the condition of the crops. Experience guides their decisions. However, a complete understanding of the impact of any decision is unknown, including the economic aspect. Combinations of weather, pests, and economic uncertainties are so numerous that it would be difficult for any person to gain sufficient experience to enable them to minimize risk in their decision making. Agricultural experimental information, such as yield response to fertilizer rates, when conducted over a several-year period at a site, usually provides the kind of information needed by professional agriculturalists who help farmers make decisions. When mean response to experiments having multiple-year and multiple levels of factors is obtained, a simple economic analysis can provide a recommended practice, given the price of output and the cost of the input. Optimum practices calculated from mean responses, however, only apply to farmers who take no account of risk. Farmers are not risk neutral. They seek goals such as (1) maximum profit or cash flow, (2) minimum variance of yield, (3) maximum stability of income, (4) minimum environmental degradation such as soil erosion and loss of nutrients or harmful chemicals to ground or surface water, and (5) some combination of the above. Crop models that use specific weather, soils, genetic, and management information can assist in evaluating strategies needed to attain farmers' goals.

Regional policy decisions related to agriculture involve maintenance of an adequate supply and quality of water for domestic and industrial consumption and a general conservation of natural resources for a region. Because agriculture is usually the major user of the water of a region, and large quantities and diversities of chemicals are applied to the land, making rational decisions regarding the impact of agricultural practices on the nonagricultural segment of society is becoming increasingly important. Because of the spatial variation in soil properties of a region and the temporal variation in weather, the use of crop models, in addition to models of other parts of the agricultural system, make the supportive decisions more rational. To establish credibility for predictions of the region however, monitoring activities will be needed at carefully selected sites to demonstrate that models predict reasonably well at those sites. Chapter 10 includes some possibilities regarding application of the model to problem solving and decision making. 

## OVERVIEW OF MODEL OPERATIONS

The model consists of a series of subroutines with a separate subroutine for each major process. In addition to this, there are subroutines associated with input and output and of the user-friendly interface. The names and functions of each of these subroutines and the interlinkages between them are indicated in the flowcharts shown in Fig. 1-5. The model uses a standardized system for model inputs and outputs that have been mutually agreed upon for the IBSNAT project (IBSNAT, 1986). The input system enables the user to interactively select crop genotypic, weather, soil, and management data appropriate to the experiment being simulated. Figure 1 flowcharts this selection process. The structure and format of all required model inputs is described in Chapter 5.

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 Fig. 2. The model uses two switches that are provided as input parameters. One of these enables the model to be run with the assumption that N is nonlimiting and thus none of the N transformation calculations are computed. The second switch 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 and execution time ubstantially. 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 (Fig. 3 and 4). A series of switches is used to route execution to different subroutines dependent upon the stage of development of the crop and whether the soil profile is draining. After these calculations are completed, output may be written to the output files (Fig. 5). The simulation continues by returning control to the point of reading the next day's weather data.

The model can be run in three modes: 

1. Single treatment simulation. This is the most common form where the inputs are displayed on the screen, the model works through the daily simulation, and then a bale showing a comparison of predicted and observed values is displayed.

2. Multiple treatment simulation. All treatments in an experiment can be simulated without requiring further inputs from the keyboard to answer the various prompts. At the end of the run all the outputs can be printed or displayed on the screen for closer examination.

3. Multiple-year run. This option is intended for cases where on wishes to examine the year-to-year variability in outcomes of a particular management strategy. For these cases outputs can be selected that provide only a single line summary for each crop season of simulation. Since all other output is bypassed, this form of model operation is the fastest.

Details on using the model are provided in Chapter 7.

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| **http://nowlin.css.msu.edu/wheat_book/CHAPTER1.htg/fig1-3.gif** |
| **http://nowlin.css.msu.edu/wheat_book/CHAPTER1.htg/fig1-4.gif** |
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# CHAPTER 2

# DOCUMENTATION OF PROCEDURES USED FOR DEVELOPMENT

# AND GROWTH WITHOUT WATER OR NUTRIENT DEFICIENCIES

## PHASIC DEVELOPMENT

The simulation of crop yield focuses around three important areas: growth duration, growth rate and the extent to which "stresses" influence these two processes. Stress can take the form of deficiencies of soil water and nutrients or extremes in temperature. The soil related deficiencies are discussed in Chapters 3 and 4. Growth duration is extremely important in the determination of potential crop yields. In general, the longer the growth duration for the crop, the higher the yield potential. In wheat, this is especially true for the period from the time the stem and inflorescence start to grow until the end of grain filling. The duration of different growth phases is referred to as phasic development. Phasic development is affected primarily by genetic and environmental factors. The genetic diversity of wheat sensitivity to photoperiod and vernalization has allowed plant breeders to select wheat cultivars that can produce grain in environments as far north as Alaska to as far south as southern Argentina and on most arable land in between where the supply of water is adequate. Because wheat has been a relatively low value crop during most of this century, it is often grown under rainfed conditions where precipitation is marginal for part or all of the season. In such instances, cultivars have to be developed that complete their life cycle soon enough to avoid complete crop failure. Because of this genetic diversity, and the diversity of regions where wheat is grown, we thought it would be essential to include quantitative aspects of phasic development in the model for it to be useful for many applications.

The CERES model separately calculates phasic development to drive the model through time. It calculates the appearance and number of leaves on the main stem, the number of tillers and the number of grains on a plant. These aspects are referred to as plant morphological development and they are calculated separately although they are closely coupled with phasic development and plant growth. Expansion growth of leaves and stems are calculated separately from mass growth because expansion growth is considered as a "sink" that is driven primarily by temperature of the expanding tissue. Mass growth is considered to be the "source" necessary to fill the expanding tissue and also provide assimilate to the root system for expansion and maintenance. Mass growth, however, is driven primarily by radiation interception by plant leaves.

By separately evaluating these four aspects of plant development and growth, the logic for partitioning assimilates into different plant parts can be accommodated according to several principles established in scientific literature. Some of the major principles include:

o During the grain filling period, the grains are the dominant sink for assimilates. Material for filling the grains can be derived from current photosynthesis and stored assimilates. Deficiencies of water and nutrients have little affect on the ability of material to be transported to the grain.

o During vegetative growth, shoots have a higher priority than roots for assimilates so long as the supply of water and nutrients from the soil is adequate. When water or nutrients are limited during vegetative growth, roots have a higher priority than shoots.

The part of the CERES model described in this chapter uses the above general principles of partitioning during different phases of development to predict the growth of a plant from a seed with particular important genetic characteristics through the many seeds at crop maturity.

The CERES-Wheat model was developed to estimate the duration of the growth cycle of different genetic types of wheat used throughout the world.  The duration of crop growth without disease, water, or pest stress is often the major determinant of crop yield potential. The relationship between biomass yield and grain yield somewhat depends on genotype, but yield is usually proportional to the above-ground biomass. Improvements in crop yield in regions of the world that have the same duration of crop growth have come mainly from improving the harvest index, i.e. the ratio of grain yield to biomass.

The major factor limiting the development of crop models for use worldwide has been in determining how the genotype of a particular crop is related to the duration of crop growth and environmental stresses.  Within any particular region of the world, crops are selected as to their ability to fit the environmental conditions of the region where they will be grown. Such adaptability relies on genetic factors, such as the ability to utilize available water, cold hardiness, and the susceptibility to winterkill.  A crop model, therefore, needs to quantify the interaction between genetic type and the environment.

Phasic development in CERES-Wheat deals with the duration of growth stages. The growth stages of wheat are organized around the plant's life cycle when changes occur in the partitioning of assimilate among the different plant organs. For example, prior to terminal spikelet formation, practically all assimilate is partitioned between the leaves and the roots. After terminal spikelet formation, stems begin to require assimilate and the ear later becomes a major site for assimilate.

In CERES-Wheat, the growth stages of wheat are numbered from 1 through 9 (Table 1). Stages 1 through 5 are the active above-ground growing stages; stages 6 through 9 describe other important events in the crop cycle. 

## PHASIC DEVELOPMENT CONTROL

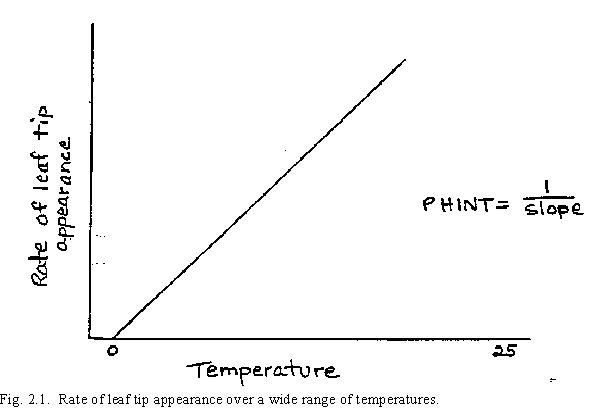
Both genotype and environment influence phasic development in CERES-Wheat. Prior to germination (Stage 9), the primary variable influencing the development rate is the soil-water environment. After

germination, the primary variable influencing the rate of development is temperature.

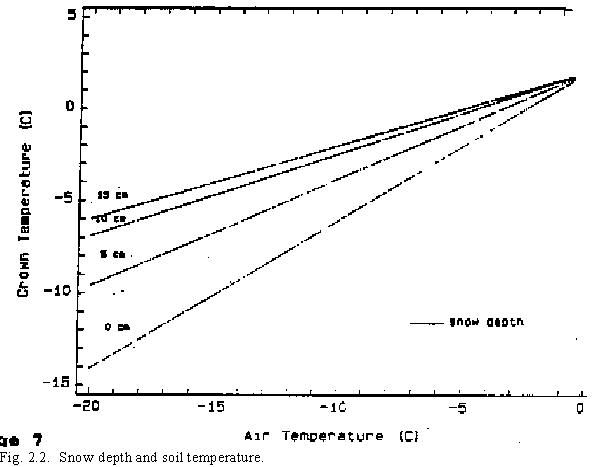
Table 1.  Growth Stages of Wheat as Defined in CERES-Wheat 

|  |  |  |
| --- | --- | --- |
| Stage | Event | Plant Parts Growing |
| 7 | Fallow or presowing | - |
| 8 | Sowing to germination | - |
| 9 | Germination to emergence | Roots, coleoptile |
| 1 | Emergence to terminal spikelet initiation | Roots, leaves |
| 2 | Terminal spikelet to end of leaf growth and beginning of ear growth | Roots, leaves, stems |
| 3 | End of leaf growth and beginning of ear growth to end of pre-anthesis ear growth | Roots, leaves, ear |
| 4 | End of pre-anthesis ear growth to beginning of grain filling | Roots, stems |
| 5 | Grain filling | Roots, stems, grain |
| 6 | End of grain filling to harvest | - |

After germination and until emergence (Stage 9), development rates are controlled by temperature. Here it is assumed that development rates are directly proportional to temperature in the range from the base temperature (0oC) to a maximum temperature of 26oC. The use of OoC as a base temperature, rather than the other base temperatures near 0oC that have sometimes been suggested, is the result from work measuring the rate of leaf appearance under controlled temperature environments. By plotting the rate of leaf tip appearance versus temperature, a near linear relationship is obtained. Fig. 2.1 demonstrates this graphically, as used in CERES-Wheat, over a wide temperature range. Extrapolating this line to a zero rate of leaf appearance intersects the temperature axis at or near 0oC. Thus daily temperature above 0oC is accumulated and referred to as thermal time (Gallagher 1979).



When the daily minimum temperature is above 0oC and the maximum is below 26oC, thermal time for a day is assumed to be the mean of the maximum and minimum values. The air mean temperature is considered to be equal to the mean temperature of the plant crown where plant expansion growth is occurring. While this assumption is subject to error for diurnal temperature variation, these errors usually cancel one another when longer period averages are used. When mean air temperatures are less than 0oC for long periods, i.e. frozen soils, the plant crown temperature is higher than the air temperature due to heat retained in the soil. When this condition occurs, a separate thermal time calculation is made. Calculating thermal time at low temperatures is especially important to determine plant hardening and freeze killing since development does not occur at temperatures less than 0oC. Snow depth also influences plant hardening and freeze killing. The insulating effect of snow at air temperatures less than 0oC raises the temperature of the plant crown higher than the air temperature--the magnitude depends on the actual snow depth[(1)](http://nowlin.css.msu.edu/wheat_book/CHAPTER2.html#N_1_) (Fig. 2.2).



**Stage 7**

Stage 7, fallow or presowing, is used to model the soil-water balance during fallow periods and is useful when the initial soil-water condition at sowing is unknown. If the initial soil-water content at

sowing is known, there is no need to run the water balance in a presowing

fallow period. If the water balance is run during the presowing period, the soil-water content can often be assumed to be either uniformly dry when the previous crop was harvested, or uniformly wet on some date following sufficient rainfall to reasonably assume wet conditions. Of course, the model requires weather information during Stage 7 runs. 

**Stage 8**

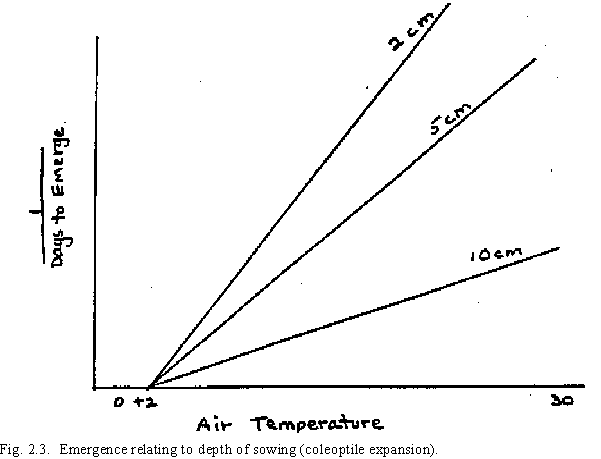
Seed germination is a rapid process and is assumed to occur in one day unless the soil water content in the top layer is near the lower limit or if the temperature is below 0oC. Under most conditions, seed would not be sown in cold soil. Seed is, however, sometimes sown in dry soil and is not expected to germinate until the soil is wet. 

**Stage 9**

Temperature and the depth of sowing are two constraints affecting seedling emergence. The soil water condition is not considered in emergence because it is assumed that if the soil water content is sufficient for germination, it is sufficient for emergence. Temperature affects emergence in the accumulation of thermal time. The affect of the depth of sowing on plant emergence is through the length of time necessary for coleoptile expansion to the surface (Fig. 2.3). The duration of Stage 9, (P9), is expressed by

P9 = 40 + 10.2 \* SDEPTH,

where P9 is the thermal time for Stage 9 and SDEPTH is the depth of sowing in centimeters, an input in the model.



**Stage 1**

Vernalization. The thermal time for all growth stages is not fixed. Vernalization, photoperiod, and genetic characteristics cause the total thermal time from, emergence to terminal spikelet, to vary considerably. Two factors determining the length of the vegetative phase of growth are leaf appearance, based only on the thermal time per leaf (PHINT), and initiation of flowering, based on vernalization and photoperiod.

Winter wheat varieties usually require exposure to relatively low temperatures before spikelet formation can begin. This low temperature requirement for flowering, called vernalization, begins at germination.

Our own phytotron work, in addition to work by others, suggests that vernalization occurs at temperatures between 0 and 15oC. The optimum temperature for vernalization is assumed to be in the range of 0oC to 7oC, with temperatures between 7oC and 15oC having a decreasing influence on vernalization. Minimum and maximum daily temperatures are used to calculate a daily vernalization effectiveness factor with a value between 0 and 1 (Fig. 2.4).  The relative vernalization effectiveness factor (RVE) is then accumulated to determine the duration of effective vernalization, or vernalization days. Vernalization days is the summation of daily RVE values. Even though there is genetic variability in sensitivity to vernalization between cultivars, fifty vernalization days are considered to be sufficient to completely vernalize all cultivars (Table 2, Fig. 2.5). The genetic variability in sensitivity to vernalization is considered by the use of a genetic specific coefficient (P1V) to calculate the influence of vernalization on Stage 1 growth. Spring wheat varieties, which have a low sensitivity to vernalization, thus can be incorporated in the CERES-Wheat model the same as winter wheat varieties by expressing the differences in vernalization through the input coefficient P1V.

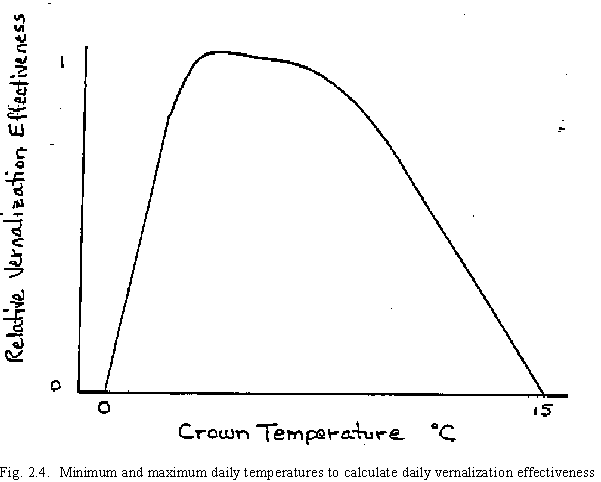
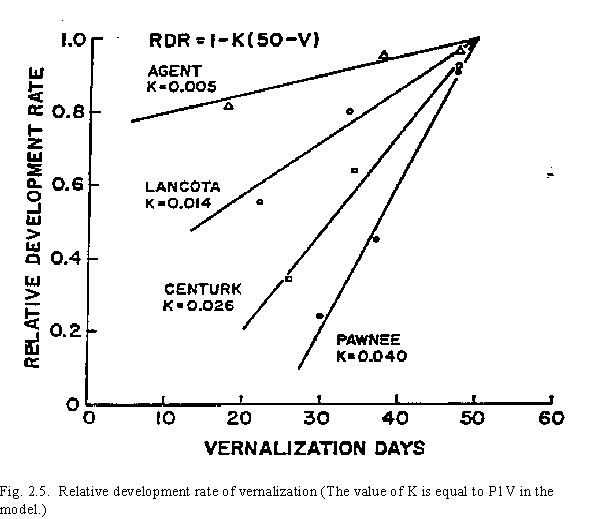


Table 2. Results of a study performed to determine coefficients for 12 varieties: values of vernalization constant (k) [RDR = 1 - k(50 - V)].

|  |  |
| --- | --- |
| Variety | k x 10-2 |
| Agent | 0.5 |
| Lancota | 1.4 |
| Centurk | 2.6 |
| Sage | 2.7 |
| Scout 66 | 2.9 |
| Sturdy | 3.0 |
| Nugaines | 3.0 |
| Triumph | 3.1 |
| Bezastaya | 3.1 |
| Coker 68-15 | 3.1 |
| Arthur 71 | 3.2 |
| Pawnee | 4.0 |

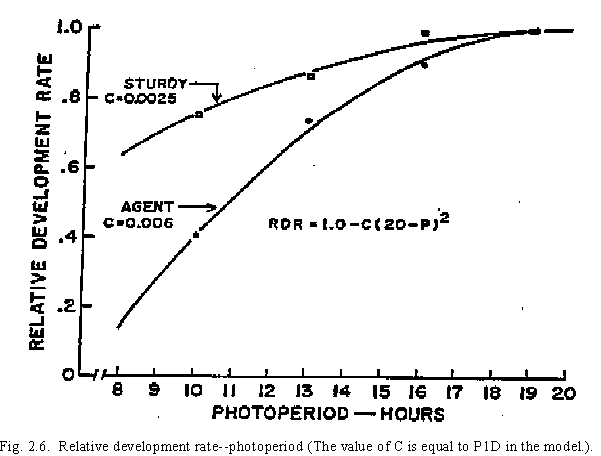


Devernalization can occur when young seedlings are exposed to high temperature. In the model, if the number of vernalization days (CUMVD) is less than 10 and the maximum temperature exceeds 30oC, then the number of vernalization days decreases by 0.5 days per degree above 30oC. If CUMVD is greater than 10, no devernalization is calculated.

A short photoperiod can delay Stage 1 plant development. In CERES-Wheat, day lengths shorter than 20 hours can delay phasic development. The delay depends on the photoperiod sensitivity of the variety being used, which is expressed in a genetic specific characteristic (P1D) (Table 3, Fig. 2.6). In the model, calculated photoperiods include civil twilight. Latitude, a required input, and the time of year are used for this calculation.

Table 3. Results of a study performed to determine coefficients for 12 variables: values of photoperiod constant (C) [RDR = 1 - C(20-P)2].

|  |  |
| --- | --- |
| Variety | C x 10-3 |
| Sturdy | 2.1 |
| Coker 68-15 | 2.6 |
| Bezastaya | 3.2 |
| Arthur 71 | 3.4 |
| Centurk | 3.7 |
| Triump | 3.9 |
| Lancota | 4.0 |
| Nugaines | 4.4 |
| Scout 66 | 4.9 |
| Pawnee | 5.2 |
| Sage | 5.5 |
| Agent | 6.0 |



Vernalization days and photoperiod are used to modify the accumulation of thermal time in Stage 1. Vernalization and photoperiod factors with values between 0 and 1, VF and DF, respectively, are calculated using the P1V and P1D coefficients. The minimum value of VF and DF is then multiplied by the thermal time to reduce rate of thermal time accumulation. When this reduced thermal time accumulation (TDU) reaches 400 degree days, Stage 1 development ends.

http://nowlin.css.msu.edu/wheat_book/CHAPTER2.htg/img.gif

where TDU = thermal development units, and DTT = daily thermal time. 

PHINT. In determining the vegetative development of wheat, it is necessary to define a term related to leaf appearance, the phyllochron. A phyllochron is defined herein as the interval of time between leaf tip appearance; in the CERES-Wheat model it is the variable PHINT. A phyllochron was assumed to be a constant number of degree days in earlier versions of the model. However, tests of models on a global scale have shown that some apparent environmental stimulus in addition to temperature causes the interval

between leaf appearance to vary. In England, winter wheat sown in the autumn has a considerably longer phyllochron (100 degree days) than spring-sown winter wheat, (75 degree days) as reported by Baker et al. 1980. The explained this phenomenon on the basis of the range of change in photoperiod. In North Dakota, wheat sown in late spring has relatively short phyllochrons, usually ranging around 75 degree days (A. Bauer, pers. comm.). Causes of this phenomenon, however, are not clearly understood and our own efforts at reproducing the effect in controlled climate chambers have

mostly failed. This, therefore, creates a degree of uncertainty in models, making an accurate prediction of crop duration difficult unless the PHINT value is known. If the sowing date for a crop is about the same time each year, the PHINT value should be constant from year to year.

The PHINT value can be measured by determining the date of appearance of leaf tips on the main stem for several plants and graphing the cumulative number of leaf tips on the Y axis against the cumulative thermal time on the X axis. The inverse of the slope of this line is the value appropriate for PHINT (see Fig. 2.7). When direct measurements of the input value of PHINT are not available, a good estimate for PHINT is 95 degree days. This value for PHINT is appropriate except for spring sown wheat in latitudes greater than 30 degrees north and 30 degrees south, in which cases a value for PHINT of 75 degree days is suggested. 

**Stage 2**

Stage 2 development, from terminal spikelet initiation to the end of leaf growth, is considered strictly under temperature control and takes 3 phyllochrons from terminal spikelet to the appearance of the flagleaf. Details of this evaluation are based on the work of E.J.M. Kirby and his co-workers at the Plant Breeding Institute in Cambridge, England. 

**Stage 3**

In Stage 3, the ear develops very rapidly and is a major sink for assimilates. At the end of this stage, the number of grains that will be filled per ear is calculated. The duration of stage 3 is the equivalent of 2 phyllochrons, even though no new leaves are appearing.

**Stage 4**

During Stage 4, the end of pre-anthesis ear growth to the beginning of grain filling, flowering takes place. Some data indicate it takes 200 degree days during this stage to go from the maximum ear size and volume to the time when linear grain mass accumulation begins. There are no apparent above-ground sinks for assimilates during this development stage in that no plant part visibly expands. The plant accumulates assimilate as stored carbohydrate during this stage for translocation to the ear during the grain filling stage. 

**Stage 5**

In Stage 5, grain filling, the size of the grain is determined. The thermal time for Stage 5 varies between genotypes and is determined by the input genetic specific constant P5. Although the thermal time is not constant for all genotypes, all values for it are near 500 degree days. This stage begins after flowering, i.e. 2 to 10 days after anthesis, with a rapid, usually linear, increase in kernel weight. 

**Stage 6**

Stage 6 is reserved for calculating the time from physiological maturity to harvest of the crop.  In the present version it is by-passed. This stage is set up for the CERES-Wheat user who needs to consider possible yield reduction problems related to an inability to harvest the crop. The details, however, are not included in the model as we could find no such dry-down model of wheat. 

## GROWTH AND ORGAN DEVELOPMENT

The purpose of the growth routine of CERES-Wheat is three-fold. The first purpose is to establish the leaf area of plants as the site of biomass production through the conversion of carbon dioxide and light energy to biomass. The second is to partition the produced biomass between the leaves, roots, stems, and ears. The last purpose, and the primary emphasis of CERES-Wheat, is to estimate grain yield as calculated by the product of the number of grains filled and their average weight.

The development of the growth routine in conjunction with the rest of the model has been a major challenge in developing this model because the partitioning of assimilate is a dynamic process, requiring several feedback mechanisms.  It is hoped that refinements will be made in the procedures developed for CERES-Wheat such that improvements in crop modeling will be realized. 

## DRY MATTER PRODUCTION

Monteith (1977) demonstrated that cumulative seasonal light interception for several crops grown with adequate soil water supply was closely related to biomass production. Although the calculated relationship for the different crops had different intercepts, there was considerable similarity. Radiation values were for those wavelengths in the photosynthetically active range and were assumed to be 50 percent of the solar radiation. Roots were included in the biomass yield even though the accuracy of the measurement of roots can be questioned. Although Monteith's results from crops in England have not been fully verified under conditions elsewhere where the radiation levels are often high, there is good reason to believe in their generality. Hesketh and Baker (1967) showed that the net photosynthesis rates of maize and cotton canopies, measured over 15 minute periods, had a nearly linear relationship to light interception.

Since studies have shown the linear relationship between biomass production and intercepted radiation, we attempted to use the constants published by Monteith (1977) to calculate biomass production in diverse regions of the world. From our results, we found that the constants obtained from that work for the conversion of intercepted radiation to biomass were too high for regions that had high daily radiation values. The field studies of Spiertz and van de Haar (1978), and Puckridge and Rathowsky (1971) demonstrated that the efficiency of conversion of intercepted radiation to biomass is greater during periods of low radiation than during periods of high radiation. This observation on the influence of radiation levels on the rate of conversion to biomass had been previously established for single leaves.

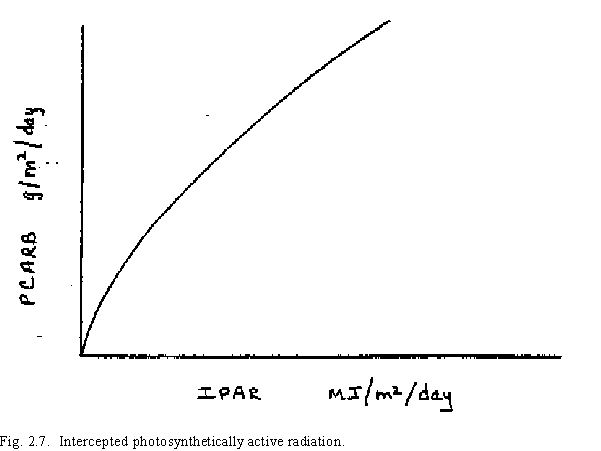
Inputs into the model for solar radiation are converted to photosynthetically active radiation (PAR), in MJ/m2/day, by multiplying the input radiation values by the constant 0.5. Use of this constant assumes that 50 percent of the incoming solar radiation is in the photosynthetically active range.

A major difficulty associated with verifying an intercepted radiation-biomass production relationship has been the lack of knowledge concerning the fraction of assimilate partitioned to the roots. Although several investigations were made to establish this relationship for use in CERES-Wheat by measuring roots or by approximating their weights compared to above ground biomass, there still remains considerable uncertainty in calculating the fraction of assimilate partitioned to the roots and tops. Several studies have reported rather large losses of the assimilate partitioned to roots through root exudations, sloughing, and other mechanisms. If these processes do indeed involve significant amounts of assimilate, then most measurements of root systems would give low estimates of the amount of assimilate transported to the roots. Because a goal of the model involved developing a reasonably representative root system, the amount of assimilate transported to the roots had to be approximately correct. To compensate for this, a somewhat higher efficiency of conversion of intercepted radiation to biomass was used than results from most field experiments have suggested.

The equation used in CERES-Wheat for potential biomass production for a given day is:

PCARB = 7.5 \* IPAR\*\*0.6,

where PCARB is the potential biomass production in grams/m2 and IPAR is the intercepted photosynthetically active radiation (Fig. 2.7).



The fraction of above-canopy radiation intercepted by the crop (IPAR) is calculated as a function of the leaf area index (LAI) by the following non-linear equation:

IPAR/PAR = 1 - EXP(-0.85 \* LAI),

where LAI is the green leaf area of the blade per plant divided by the land area occupied by the plant.  The value for LAI is calculated in another section of the growth routine based on an initial LAI value at emergence of 0.4 cm2. After the first day, the value for LAI comes from daily leaf expansion calculations.

Some investigators have appropriately included the area of leaf

sheaths exposed to light in the LAI. We assume that the proportion of sheaths exposed to light compared to the leaf blade area is a constant. Thus blade area is used for simplicity. The apparent extinction coefficient of 0.85 used in the intercepted radiation equation, therefore, is higher than some published extinction coefficients. This higher value offsets the smaller LAI value that results from using only blade area for the LAI. Although it was difficult to arrive at a precise value for the extinction coefficient, a sensitivity analysis using the range of values for the extinction coefficient suggested by others, 0.65 to 0.95, indicated that the accuracy of the extinct coefficient was not a critical factor in determining IPAR unless LAI values less than 1.5 persisted throughout a season.

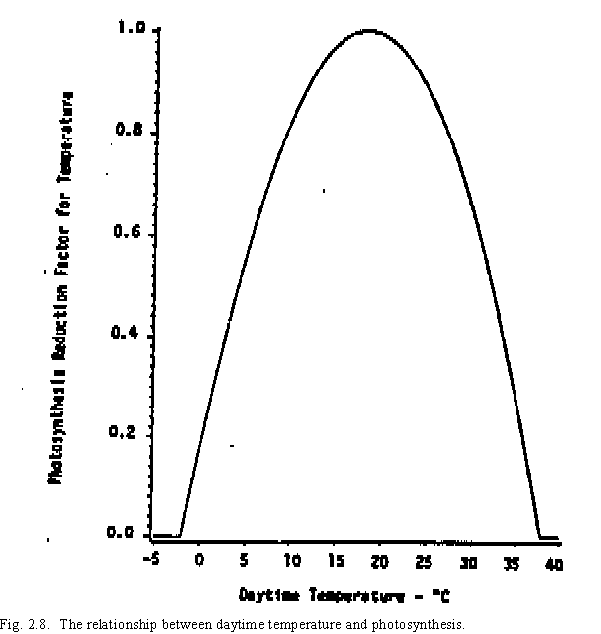
Two factors can reduce potential biomass production:  non-optimal temperatures and water stress. A weighted daytime temperature is calculated from the minimum (TEMPMN) and maximum (TEMPMX) daytime temperatures for use in the photosynthesis temperature reduction factor (PRFT), where the optimum daytime temperature is considered to be 18`C. The daytime temperature (T) is approximated by the relationship

T = 0.25 \* TEMPMN + 0.75 \* TEMPMX,

The reduction in photosynthesis due to temperature is then

PRFT = 1 - 0.0025 \* (T - 16)\*\*2,

for all values of PRFT greater than or equal to 0 (Fig. 2.8).  Values obtained for PRFT that are less than 0 are set equal to 0..



Water stress reduces dry matter production rates below the potential whenever crop extraction of soil water falls below the potential transpiration rate calculated for the crop. This reduction factor, SWDF1, is calculated in the water balance sub-routine outlined in Chapter 3 and is used with PRFT to calculate the actual biomass production. The actual biomass production (CARBO) is thus determined by the equation

CARBO = PCARB + [min(PRFT,SWDF1)].

Respiration rates are assumed to be proportional to the carbon fixed by photosynthesis and are not calculated independently, but rather incorporated into the calculation of PCARB and PRFT.

The remainder of the growth component of the model involves the partitioning of assimilate during the five phasic development stages. For this development, CARBO is converted to a per plant basis by dividing CARBO by PLANTS, the plant population per square meter. Thus, a single plant growing in competition with other plants is modeled.  We assume that all plants for the area being modeled are homogeneous. 

## LEAF GROWTH AND TILLERING

Plant leaf area has an important influence on light interception and dry matter production. The rate of leaf area expansion is a component of plant growth that is quite sensitive to environmental stresses. For example, leaf expansion growth is more sensitive to plant water deficits than is photosynthesis. Thus drought stresses reduce leaf expansion growth more than they reduce photosynthesis. This reduction in expansion growth without a concomitant photosynthesis decrease can increase the specific leaf weight or increase the proportion of assimilate partitioned to the roots. The model accounts for these plant responses by using separate water deficit functions for reducing leaf expansion growth and photosynthesis.

The daily increase in plant leaf area results from the growth of leaves on both the main stem and the tillers. In the model, the area of the leaves on the main stem is first calculated; then an adjustment then is made for the number of tillers on the plant. 

## DEVELOPMENT OF MAIN STEM LEAF AREA

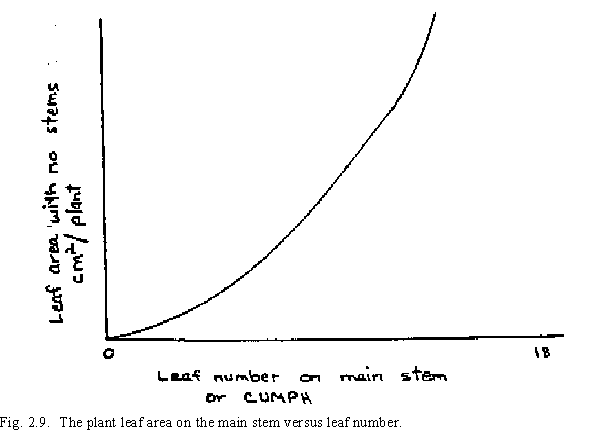
The leaf area of a plant is the product of the rate of leaf appearance and the rate of expansion of the growing leaves. When only blade area is considered, we assume that only one leaf at a time is expanding on a stem during vegetative growth. Kirby et al. (1982) has shown that while two leaves are in an active expansion stage, only one of these leaves is contributing new, visible growth. The growth of the other leaf occurs within the sheath of the uppermost visible leaf and does not contribute to the leaf area available to intercept solar radiation.

The leaf appearance rate is a linear function of temperature between the range of about 0oC and 26oC (Fig. 2.1). Thus leaves appear at predictable intervals using known temperature information. The leaf appearance interval, PHINT, is also used as a basis for determining leaf area growth. Both the rate of appearance and the rate of leaf expansion are assumed to be controlled by temperature in the same way. Thus, leaf area growth rate can be calculated as a function of temperature without separately considering the individual leaf appearance and expansion rates.

The expansion rate of the first leaves on the plant is less than that of the later leaves due to the ability of the plant to acquire the assimilate to support larger leaves after more green leaf area is present. The first leaves of the plant, therefore, are smaller (Fig. 2.9). The plant leaf area growth rate on the main stem (PLAGMS) is determined from the following equation:

PLAGMS = 7.5 \* CUMPH\*\*0.5 \* TI, in cm2/day,

where CUMPH = cumulative phyllochrons since emergence, and TI = DTT/PHINT, the daily phyllochron fraction.



From the main stem plant leaf area growth rate, a first approximation of the total plant leaf area growth rate (PLAG) can be determined.

PLAG = PLAGMS \* TILN,

where TILN = the number of tillers/plant. The calculations for tiller number will be discussed in a later section.

To convert the leaf area growth rate into values describing the mass of growth obtained, we considered the only constraints on the potential leaf area growth to be a soil water deficit, which is imposed regardless of competition. This soil water deficit, SWDF2, is obtained from the soil water balance routine.

To determine the amount that leaves can grow, the leaf area to weight of assimilate ratio (AWR) is first calculated. The AWR in Stage 1 includes all of the above-ground biomass of the plant, which only consists of leaves, since the stem has a negligible contribution to the plant biomass in Stage 1. The AWR for Stage 1, early vegetative growth, is described by the equation

AWR = 150 - 0.075 \* TDU.

Although AWR can change more than the above equation implies, we found it difficult to allow AWR to vary with the environmental conditions along with other dynamic factors affecting partitioning. If AWR varies with environmental conditions, then it is difficult to control tillering development.  Therefore in Stage 1, the model does not allow AWR to vary except with the aging of the plant. This is, however, only a consideration for Stage 1 growth since AWR is not used after Stage 1.

The potential leaf growth (GROLF) is the mass of assimilate required to support that amount of daily expansion growth in the plant and is expressed by

GROLF = PLAG/AWR, in gm/plant.

The root growth is then assumed to consist of the remainder of the daily assimilate supply.

GRORT = CARB - GROLF.

If the root growth is more than 35 percent of CARBO in stage 1 growth, the plant is assumed to have an adequate assimilate supply for leaf growth to proceed at its potential rate (Gregory et al. 1978b). If GRORT is less than 35 percent of CARB, then GROLF is reduced such that its value is 65 percent of CARB and GRORT is therefore 35 percent of CARB. When this happens, a new value for PLAG is determined by

PLAG = GROLF \* AWR.

The total cumulative plant leaf area (PLA) is then updated by adding the daily growth:

PLA = PLA + PLAG.

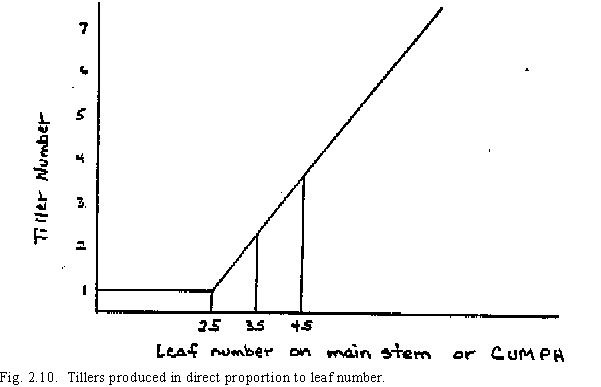
The above considerations are used to account for the competition for assimilate between the main stem and the tillers.

Early in Stage 1, seedlings have a reservoir of carbohydrate available for leaf and root growth in the seed endosperm. The model supplements the supply of assimilate with the carbohydrate from seed storage until the seed endosperm storage capacity is depleted. 

## TILLERING

The total potential rate of tiller formation depends on the thermal time after emergence, as contained in the concepts developed earlier for cumulative leaves developed or cumulative phyllochrons (CUMPH). After three phyllochrons, tillers are assumed to be produced in direct proportion to the leaf number (Fig. 2.10),

TC1 = -2.5 + CUMPH.



Although the rate of subsequent tiller formation by the main stem tillers would also follow this relationship, the actual number of potential tillers formed is limited by the available assimilate. This competition for assimilate between tillers is evaluated using the number of tillers per square meter (TPSM), where

TPSM = PLANTS \* TILN

where PLANTS is an input plant population. A rate of tiller formation based on the competition limitations of tillers per square meter is calculated:

TC2 = 2.56E-10 \* (2500 - TPSM)\*\*3.

The number of tillers per plant (TILN) is updated by the rate of daily tiller formation and is calculated as:

TILN = TILN + TI \* min(TC1, TC2),

where TI = DTT/PHINT, the daily phyllochron fraction. For early tiller growth, TC1 is usually the minimum for the rate limiting function. As more tillers are formed, the rate calculated for TC2 is usually the minimum due to increased competition.

A water deficit factor can reduce tillering factor similar to the leaf growth rate, based on SWDF2 from the water balance routine.

If stresses or competition cause TILN to be less than one, it is assumed that the plant population does not decrease. If TPSM is greater than 1000 at the end of Stage 1 growth, TILN is reduced to 1000/m2. This is needed logically for later calculations and is based on the observation that no more than 1000 tillers/m2 would be able to produce ears. The reduction is needed during Stage 2 development where a reduction in tiller number due to assimilate competition is considered. 

## LEAF SENESCENCE

Leaf senescence is primarily coupled to plant leaf development. Several investigators have observed that each stem maintains only about four green leaves. Assuming that no other stresses cause early leaf senescence, senescence begins in the oldest leaves after four leaves have been formed. The plant maintains the four newest leaves as green leaves while the other leaves senesce. This type of senescence can be explained by both the shading of the older, lower leaves, by the upper, newer leaves, and by physical damage received by the older leaves as a result of stem expansion and leaf sheath splitting.

The plant leaf area loss rate (PLALR) is determined by

PLALR = [PLSC(LN - 4) - PLSC(LN - 5)] \* TI,

where PLSC is the cumulative leaf area at the time when each main stem leaf reaches full size, LN is the leaf number on the main stem accumulated since emergence, and TI is the daily phyllochron fraction.

From the above relation, the senescence leaf area (SENLA) is determined,

SENLA = SENLA + PLALR.

When soil water deficits are present, the plant leaf area senescence is increased by a factor related to SWDFI. From the plant leaf area PLA and SENLA, we now determine the green leaf area index, LAI.

LAI = (PLA - SENLA) \* PLANTS \* 0.0001,

where the constant 0.0001 converts leaf area units from cm2 to m2. The equations used to calculate senescence xx are used throughout the life cycle of the crop. Thus, when PLA reaches its maximum value at the end of leaf growth, senescence causes a gradual decline in LAI.

## STEM GROWTH (Stage 2)

In the course of Stage 1 development, the number of tillers developed usually exceeds the number of tillers that can eventually develop stems and ears. Thus, the potential assimilate sinks exceed the supply. Under such conditions, the major challenge in the model becomes the proper partitioning of the available assimilate between stems, leaves and roots. The partitioning of the assimilate to the non-root parts of the plant is expressed by the relationship

PTF = 0.7 + SWDF1 \* 0.1,

where PTF = the top fraction of the plant. Thus PTF equals 0.8 under conditions of no water stress and 0.7 when conditions of the most severe water stress exist. After the assimilate is partitioned to the top portion of the plant, the remainder is allocated to the roots. Unlike Stage 1, in Stage 2 there is no minimum threshold percent of the assimilate obligated to be partitioned to the roots. Once PTF is determined, that fraction must be partitioned between the stems and the leaves.

After terminal spikelet formation at the end of Stage 1, the fraction of assimilate partitioned to the stem gradually increases from practically none to about 0.5 by the end of Stage 2. The rate of all stem growth, including tillers (GROSTM), is expressed by the following equation:

GROSTM = (0.15 + 0.12 \* DTT/PHINT) \* CARBO \* PTF.

The rate of leaf growth (GROLF) is then determined:

GROLF = CARBO \* PTF - GROSTM.

During Stage 2, the new leaf area is considered to be proportional to the new leaf weight. This proportionality constant, 115 cm2/gm, assumes only leaf blade area while the leaf weight includes both leaf blades and sheaths. The total leaf area (PLA) is then updated,

PLA = PLA + GROLF \* 115.

## TILLER DEATH

Tiller death is considered to result from an insufficient supply of assimilate to support tiller growth and maintenance. The assimilate demand by a single tiller is calculated, assuming that this demand is proportional to the rate at which the stem elongation can occur. This single stem elongation rate can vary considerably between plant genotypes. Dwarf or semi-dwarf genotypes have less demand per stem than genotypes with large stems. The rate of potential biomass gain for a single tiller is determined from thermal time and the weight of a single tiller (TILSW) updated by the following equation:

TILSW = TILSW + G4 \* 0.0089 \* DTT \* SUMDTT \* SWDF1/PHINT\*\*2,

where G4 is the genetic specific constant (gm/stem). The constant G4 is by definition the final potential dry weight for a single stem plus ear at anthesis when the crop has grown under optimum conditions.

Once the single tiller demand for assimilate is determined, logic in the model provides a time-delayed balance with the assimilate supply to determine the number of tillers that can elongate under the assimilate constraints. This is accomplished by deriving a daily ratio (RTSW) between total plant stem weight and the potential plant stem weight if all tiller (TILN) stems could be the weight of the calculated single tiller TILSW.

RTSW = STMWT/(TILSW \* TILN),

where STMWT is the total plant stem weight. The time delayed reduced tiller number is updated with the equation

TILN = TILN - [TILN \* DTT \* 0.005 \* (1 - RTSW)]

## PREANTHESIS EAR GROWTH (Stage 3)

During Stage 3 development, plant growth continues to the end of preanthesis ear growth and has a duration that is the equivalent of two phyllochrons. The major growing parts during this period are the stem, ear, and roots. Because of the difficulty of knowing exactly when the major portion of ear growth is initiated and its relatively short expansion period, we do not distinguish between the weight of ear and the stem. In the model their weights are combined in the variable STMWT.

The fraction of daily assimilate partitioned to the top parts of the plant (PTF) is assumed constant unless there is a soil water deficit. The partitioning of assimilate to the non-root parts of the plant is similar to that used for stem growth in Stage 2 development,

PTF = 0.75 + SWDF1 + 0.1.

This equation reflects a 5 percent increase in the portion of assimilate partitioned to the top parts of the plant as compared to Stage 2 development. The range of PTF is from 0.85 under conditions of no water stress to 0.75 under conditions of the most severe water stress. Similar to Stage 2 development, after the assimilate is partitioned to the top portion of the plant, the remainder of the assimilate is allocated to the roots.

The rate of potential biomass gain for a single tiller during Stage 3 is a linear function of thermal time multiplied by G4. Single tiller weight (TILSW) is updated by this rate

TILSW = TILSW + G4 \* DTT \* 0.25/PHINT \* SWDF1.

Similar to Stage 2 development, the single tiller assimilate demand is balanced against the assimilate supply and a reduction in tiller number is possible.

TILN = TILN -[TILN \* DTT \* 0.005 \* (1 - RTSW)].

At the end of Stage 3 the minimum stem weight (SWMIN) is calculated. This value is assumed to represent the minimum stem weight that can occur when the stem reserve assimilates are used during grain filling. When the potential grain growth rate of the plant is such that the assimilate from photosynthesis is not sufficient to meet this demand, the stem carbohydrate reserves are used to meet this demand. When this occurs, the stem weight may decrease, but only to the minimum stem weight.

The plant leaf area reduction rate (PLALR) due to senescence in Stage 3 is:

PLALR = 0.0003 \* DTT \* GPLA,

where GPLA is the plant green leaf area (PLA - SENLA) at the end of Stage 2.

The senescence leaf area is then updated

SENLA = SENLA - PLALR.

## END OF EAR EXPANSION TO THE BEGINNING OF GRAIN FILLING (Stage 4)

Stage 4 development has a duration of 200 degree days. During this stage, the plant has no above ground organs that actively expand. Carbohydrates are stored during this stage giving rise to an increase in stem weight. This reserve carbohydrate can later be transported to the grain. Stage 4 is important in establishing the grain yield because the stem plus ear weight at the end of this is assumed to be proportional to the number of grains that can be filled. Anthesis also occurs during this stage.

During Stage 4, 90 percent of the daily biomass produced is assumed to be partitioned to the plant top unless there is a water stress. Under conditions of water stress, this can be reduced to 80 percent.

PTF = 0.8 + SWDF1 \* 0.1.

We assume for simplicity that during stage 4 all of the weight increase in the plant top occurs in the stem and ear.

The plant leaf area loss rate () and the senescence leaf area (SENLA) are calculated for stage 4 development similar to that for stage 3, except that the rate is somewhat faster due to plant aging.

PLALR = 0.0006 \* DTT \* GPLA.

Water stress can increase the senescence rate. The updated leaf senescence is

SENLA = SENLA + PLALR.

At the end of Stage 4, the base temperature for thermal time determination is changed from 0 to 1 for the subsequent thermal time determination in Stage 5. The number of kernels per plant (GPP) is assumed to be the product of the total stem plus ear weight at the end of Stage 4 times a genetic specific constant, G2. This constant is used to account for varietal differences in the number of kernels produced per ear.

GPP = STMWT \* G2.

The value obtained for GPP from this calculation is not altered during the remainder of the plant's life cycle unless severe water stresses cause the abortion of some of the grains during the grain filling stage. 

## GRAIN FILLING (Stage 5)

We had difficulty in establishing the rate of photosynthesis for plants during grain filling when the leaves are aging. Root growth usually is negligible, and most data indicate that some of the assimilate used for grain filling comes carbohydrates stored in other plant parts. Most measurements of total above ground biomass production rates during the grain filling stage indicate a decline relative to earlier growth rates. Furthermore, an increase in maintenance respiration due to larger plant size should occur at this time. The assumption throughout all growth stages is that respiration is proportional to gross photosynthesis as altered by the temperature reduction factor discussed earlier. During this stage, this assumption may not be as valid as for the other stages.

The rate of photosynthesis could depend on the actual demand for assimilates during grain filling (Evans et al. 1975). Another possibility is that more assimilate is partitioned to the roots when the demand for grain filling is low. With these dynamic feedback mechanisms and the uncertainty of the amount of translocation to the grain, the scaling of daily photosynthesis was difficult. To estimate the amount of assimilate derived from photosynthesis and the amount from storage carbohydrate, the following relationships were used. The plant top fraction, PTF, during this stage is

PTF = SWMIN/ STMWT \* 0.35 + 0.65,

where SWMIN is the minimum stem weight calculated at the end of stage 3 and STWMT is the stem weight. This allows more mass to be partitioned to the roots when there is a large supply of stored carbohydrates in the plant top.

When the stored carbohydrate has been used, all of the assimilate from photosynthesis then goes to grain filling, i.e. when SWMIN = STMWT. The range for the value of PTF is usually between 0.7 at the beginning of Stage 4 and to 1.0 at the end. As in other stages of development, the roots are assigned the fraction of assimilate not partitioned to the plant top fraction.

The rate of photosynthesis as influenced by aging of the leaves and sink assimilate demand is approximated using an equation that reduces the original calculated value of CARBO.

CARBO = CARBO \* (1 - (1.2 - 0.8 \* SWMIN/STMWT)

\* (SUMDTT + 100)/(P5 + 100)),

where P5 is the duration of grain filling in degree-days. The leaf aging affect is determined by the (SUMDTT + 100)/(P5 + 100) ratio in the equation and the sink demand is inferred indirectly through the SWMIN/STMWT ratio. This relationship is shown graphically in Fig. 2.11.

Senescence in Stage 5 is determined by a non-linear equation which considers the plant leaf area loss rate (PLALR) as the plant approaches maturity.

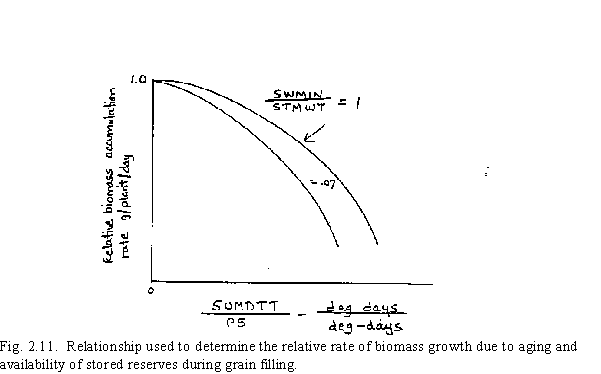
PLALR = GPLA \* 2 \* SUMDTT/P5\*\*2.

The kernel growth rate in Stage 5 is calculated on a single kernel basis and assumes that all kernels grow at the same rate. First a relative kernel filling rate is calculated as a function of temperature. The grain filling rate is assumed to be proportional to temperature between 0 and 17oC, with an optimum plateau temperature for rain filling above 17oC. If the mean temperature is less than 10oC, then the rate of grain filling (RGFILL) is determined by the equation

RGFILL = 0.065 \* TEMPM,

where TEMPM is the mean temperature and the rate of grain filling is not allowed to be less than 0. When the mean temperature is greater than 10oC,

RGFILL = 0.65 + (0.0787 - 0.00328 \* (TEMPMX - TEMPMN)) \* (TEMPM - 10)0.8.



The value of RGFILL is not allowed to exceed 1.

During grain filling plant water deficits only influence grain filling through the reduction in assimilate supply.

The daily whole plant potential grain growth (GROGRN) is calculated from the relative grain filling rate, the number of grains per plant, and the genetic constant G3.

GROGRN = RGFILL \* GPP \* G3 \* 0.001,

where RGFILL is the actual grain filling rate, GPP is the kernels per plant, G3 is a genetic specific kernel growth rate constant, and 0.001 is a factor to convert units mg to g.

To calculate the actual rate of daily grain growth, it is necessary to determine if the photosynthesis plus stored assimilate supply is adequate to support the growth of all of the kernels. To do this, the value of GROSTM is calculated by adding the plant top biomass and subtraction of the potential grain growth.

GROSTM = CARBO \* PTF - GROGRN.

Depending on the state of carbohydrate reserves in the stem and the daily assimilate supply, the value of GROSTM may be either positive or negative. The updated stem weight is then calculated.

STMWT = STMWT + GROSTM

If STMWT is greater than or equal to SWMIN, then the rate of kernel growth is equal to the calculated potential rate. If STMWT is less than SWMIN,

no further carbohydrate is available and grain the filling rate is equal to the daily biomass partitioned to the plant top. This reduction in grain growth usually only occurs near the end of the grain filling stage because the stored carbohydrates are depleted and the daily assimilation rate is low because of the reduction in green leaf area due to senescence.

The plant grain weight, (GRNWT) is updated by the actual grain growth rate (GROGRN).

GRNWT = GRNWT + GROGRN.

The dry weight yield per unit area at the end of Stage 5 is calculated by multiplying the grain weight per plant, GRNWT, by the plant population, PLANTS. This yield calculated in the model is then corrected to include a grain water content of percent. If, at the end of grain filling, water stress prevented individual kernel weights from attaining a weight of 20 mg, then the individual kernel grain weight is assumed to be 20 mg and the kernel number is reduced to provide the calculated whole plant grain weight. This is done to accommodate the observation that some grains are aborted during severe drought while other grains remain relatively small but viable. 

## DEVELOPMENT OF THE ROOT SYSTEM

Root length density is needed to calculate root water absorption and to evaluate the soil water deficit factors that decrease various plant processes.

Throughout each stage of plant development, some assimilate was partitioned to the roots (GRORT). To simulate a root absorbing system it is necessary to convert root mass (GRORT) to root length. To account for biomass losses due to root exudations and sloughing, we assume that only 60 percent of the biomass partitioned to the roots is actually involved in structural root weight gains. Furthermore, an additional 0.5 percent of the root mass is assumed to be lost daily through respiration. The root weight is not, however, directly used in the model and is included with the model output for those interested in comparing the model result with field measurements. The conversion of GRORT to root length is based on the data of Gregory et al. (1978a)that there is about 1.05 X 104 cm root length per gram of root. Based on this approximation the daily new root length (RLNEW) is

RLNEW = GRORT \* PLANTS \* 1.05,

where 1.05 is a constant that converts the daily biomass partitioned to the roots of an individual plant to cm of root length per cm2 of soil.

Because the model is not three dimensional in soil space, the root length calculations assume that the roots are equally distributed throughout the soil area. This assumption is not valid for young plants whose roots are concentrated near the seed. In some instances this model assumption can cause erroneous predictions.

The downward movement of roots is assumed to be proportional to the daily thermal time in the same way that leaf development is affected. Exceptions to this are when the soil is dry at the level where the roots are growing downward or when the plant itself is under water stress. When no stresses are considered, the downward rate of root growth is assumed to be 0.22 cm/degree-day. The downward rate of root growth is used to update

root depth (RTDEP)

RTDEP = RTDEP + DTT \* 0.22 (min(SWDF1 \* 2, SWDF),

where SWDF1 is a plant stress factor determined in the soil water balance routine, and SWDF is a water stress factor for the soil level where the roots are growing. The factor SWDF has a value of 1 when there is at least 25 percent of the total extractable soil water (ESW) at the depth where the roots are growing. If the ESW is less than 25% of then

SWDF = 4 \* (SW(L) - LL(L))/ESW(L),

where SW(L) is the water content at the depth increment (L) where the roots are growing, LL(L) is the lower limit of extractable water at that level, and ESW(L) is the difference between the drained upper limit soil water content (DUL(L) and LL(L). The limits of the soil water content at a particular soil level are discussed more fully in Chapter 3.

The distribution of the roots within the soil layers is evaluated by calculating a relative root length density factor (RLDF) at each soil depth increment (DLAYR(L)) where the roots are growing

RLDF(L) = SWDF \* WR(L) \* DLAYR(L),

where WR(L) is a root preference factor for each layer (L).

The root preference factor WR(L) is a soil input for each depth increment that depends on soil properties and ranges in value from 0 to 1. It represents the relative preference for root growth at the different depths if the soil water content and nutrient level are not below threshold values.

Several factors affect the distribution of roots at various soil depth levels. Model root formation occurs at the crown of the plant, usually causing a higher density of roots near the surface. Also, the upper soil levels generally contain higher amounts of nutrients and organic matter, causing more roots to develop there. The upper soil layers are also usually more easily penetrated by roots because they have been disturbed by tillage.

To obtain the distribution of new root growth with depth, a root length density factor (RLDF(L)) is calculated for each soil depth increment down to the lower boundary of the root zone (RTDEP).

RLDF(L) = WR(L) \* DLAYR(L) \* MIN (SWDF, RNFAC),

where MIN indicates that the computer will select the minimum value of the variables that are given in the parentheses. The value of SWDF is a limitation on root growth due to water shortage in a layer and has already been defined for root depth routines and RNFAC is a limitation on root growth due to nitrogen shortage. As with SWDF, RNFAC has a value ranging from 1 for no limitation to near 0 for a strong limitation on root growth.

RNFAC = 1.0 - (1.17 \* EXP (-0.15 \* TOTN))

where TOTN is the total nitrogen in the layer under consideration. Details on the nitrogen dynamics calculations are provided in Chapter 4.

The sum of the values of RLDF(L) for each layer with roots is calculated as a total root length density factor TRLDF. The fraction of new root growth at each soil depth then becomes RLDF(L)/TRLDF. The root length density RLV(L) for each depth increment is then updated.

RLV(L) = RLV(L) + (RLDF(L)/TRLDF) \* (RLNEW/DLAYR(L)) - 0.01 \* RLV(L).

where the last term calculates a one percent reduction in RLV(L) to account for root loss by death, sloughing, and other factors. The value of units of RLD(L) are cm root length per cm3 of soil.

1. The primary data for this conclusion was provided by Dr. K. Aase from unpublished results obtained at Sydney, Montana. Aase measured the soil temperature at 2 cm and the air temperature at 2 m.

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# CHAPTER 3

## SOIL WATER BALANCE

The effect of soil and plant water deficits on plant growth and yield reduction is calculated by the soil water balance. The soil water balance routine of CERES-Wheat includes the soil water quantity resulting from the input of precipitation and irrigation, the outputs of evaporation from plants and the soil, and runoff and drainage. In the model, the soil water balance is distributed in up to ten layers. The user assigns the depth of each layer. The water balance routines described in this chapter were not designed to be accurate for wetlands where a water table is present near the surface nor where artificial drainage occurs. It was primarily developed to evaluate naturally drained soils where shortages in the soil water balance are likely to occur, not where aeration problems may reduce crop growth.

The water content of any particular soil layer can decrease as a result of soil evaporation, root absorption, or water flow to an adjacent layer. The limits to which water can increase or decrease are inputs for each soil layer. These limits are the lower limit of plant water availability (LL(L)), the field drained upper limit (DUL(L)), and the field saturated water content (SAT(L)). When the crop water supply is marginal, the accuracy of these input limits becomes quite important for accurate prediction of crop performance.

Traditional laboratory measurements of wilting point and field capacity water content are frequently inaccurate for establishing field limits of water availability (Ritchie 1981). Field measurements are preferred when possible. A comparison of field-measured versus laboratory-measured limits of soil water content values taken from several sites in the United States revealed that considerable error was possible when laboratory methods were applied to the field limits (Ratliff et al. 1983).

Other soil inputs needed in the model include the soil albedo (SALB), the upper limit of first stage soil evaporation (U), a constant for calculating the drainage rate (SWCON), and a curve number used to calculate run-off (CN2).

If irrigation water is applied to the field being simulated, then the day of the year of irrigation (JDAY(J)) and the amount of irrigation (AIRR(J)) are read for the number of irrigations (NIRR) specified in the data. When the soil water balance routines begin on the date specified by the beginning of weather data, several variables have to be initialized with some reasonable logic. This initialization is done in the subroutine where soil properties are read from a file and initialized (SOILRI).

## INITIATION OF PARAMETERS

First, the ratio of actual to potentially-extractable soil water (SWR) is calculated for layer 1 (the upper layer) by the following equation:

SWR = ((SW(1) - LL(1))/(DUL(1) - LL(1)),

where SW(1) is the initial soil water content of layer 1, LL(1) is the lower limit of plant-extractable soil water at layer 1, and DUL(1) = the drained upper limit of layer 1. SWR is then used to initialize the cumulative stage 2 soil evaporation (SUMES2).

If SWR is less than 0.9, then

SUMES2 = 25 - 27.8 \* SWR,

and the cumulative stage 1 soil evaporation (SUMES1) is set equal to the upper limit of stage 1 soil evaporation (U). The time after the beginning of stage 2 evaporation (T) is then calculated.

T = (SUMES2/3.5)\*\*2.

If SWR is greater than 0.9, then both SUMES2 and T are set to 0 and the cumulative stage 1 soil evaporation (SUMES1) is calculated from the equation

SUMES1 = 100 - SWR \* 100.

These evaporation parameters come from the published model of Ritchie (1972).

The initiation subroutine then calculates the plant-extractable soil water (ESW(L)) for each layer

ESW(L) = DUL(L) - LL(L).

for use in output information and some calculations within the model.

The initialization program also calculates the cumulative depth of the soil profile (CUMDEP), the total soil water in the profile (TSW), the total plant-extractable soil water (TPESWP), the total soil water in the profile at the lower limit of plant extractable water (TLL), the total soil water in the profile at the drained upper limit (TDUL), and the total soil water in the profile at saturation (TSAT). These are used only to provide a printed output for users to quickly summarize the soil properties.

A weighting factor used to modify runoff curves numbers with near surface soil condition (WF(L)) is calculated from the equations

WX = 1.016 \* (1 - EXP(-4.16 \* CUMDEP/DEPMAX)),

and

WF(L) = WX - XX,

where XX is equal to 0 in the top layer, i.e. WF(L) = WX. In the other layers, XX is equal to the WX calculated for the layer above.

The intermediate variables used to calculate the run-off, CN1 and SMX, are calculated from the input curve number CN2.

CN1 = -16.9 + 1.348 \* CN2 - 0.01379 \* CN2\*\*2 + 0.0001172.

SMX = 254 \* (100/CN1 - 1).

Details of the runoff procedures are discussed in the next section.

## INFILTRATION AND RUNOFF

Daily precipitation in mm is input into the model from the weather data file. If irrigation and/or precipitation occur on a day, the amount of irrigation (AIRR(J)) and precipitation (RAIN) are summed. The water balance subroutine calculates run-off by a modification of the USDA-Soil Conservation Service (SCS) curve number method (Williams et al. 1983). The SCS procedure uses the total precipitation from one or more storms which occur in a single day to estimate run-off, and excludes time as an explicit variable, i.e. rainfall intensity is ignored.

While the SCS procedure utilizes antecedent rainfall amounts to determine soil wetness and run-off, the procedure of Williams et al. for layered soils considers the wetness of the soil in the layers near the surface. This is accomplished by first calculating a sum (SUM), weighted for soil depth by the factor WF(L), of the relative amount of plant-extractable soil water in the profile. The SCS curve number retention parameter (R2) is then calculated from SUM and the maximum value of R2 (SMX):

R2 = SMX \* (1 - SUM),

where R2 cannot be less than 2.54 mm. The value SMX was calculated in the SOILRI subroutine.

Fig. 3.1 illustrates the SCS curve number concept with variations which allow for wet or dry conditions near the surface. The run-off curve concept is not expected to provide accurate run-off and infiltration information for a specific storm. The curve number concept was empirically derived to approximate the run-off volume when only daily rainfall is known. If a greater accuracy is required, a more physically based approach would be required. Such an approach would have to include information regarding storm intensities. Because storms vary both spatially and temporally, accurate modeling of infiltration and run-off would require more frequent rainfall measurements than daily values. These measurements would have to be taken in a dense network to provide spatially balanced input information. The knowledge of the right rainfall values for a particular site where the model is to be applied is one of the limiting factors affecting model accuracy.

Fig. 3.1. SCS curve number concept.

No run-off occurs if the temporary variable PB is less than zero, where

PB = PRECIP - 0.2 \* R2.

If run-off does occur, then infiltration is calculated as the difference between precipitation and run-off.

PINF = PRECIP - RUNOFF.

**DRAINAGE**

Water can be taken up by plants while drainage is occurring. Thus the drained upper limit soil water content is not always the appropriate upper limit of soil water availability. Many productive agricultural soils drain slowly, providing a possibly significant quantity of water to plants before drainage practically stops. In CERES-Wheat, the redistribution of water in the soil profile and drainage out of the rootzone are calculated using a functional model developed from field drainage information.

Using a cascading approach, water is moved downward from the top soil layer to lower layers. Drainage from a layer takes place when the soil water content (SW(L)) is between field saturation (SAT(L)) and the drained upper limit (DUL(L)).

For drainage calculations, the infiltration PINF is converted from mm to cm and a downward flux for each layer calculated (FLUX(L)). This information is needed for calculating leaching. When FLUX(L) is not equal to zero, the amount of water that the layer can hold (HOLD) between the current volumetric water content (SW(L)) and saturation (SAT(L)) is calculated.

HOLD = (SAT(L) - SW(L)) \* DLAYR(L).

If FLUX(L) is less than or equal to HOLD, an updated value of SW(L) is calculated prior to drainage.

SW(L) = SW(L) + FLUX(L)/DLAYR(L).

If this new SW(L) is less than the drained upper limit of volumetric soil water in the layer (DUL(L)), no drainage occurs. If this SW(L) is greater than DUL(L), drainage (DRAIN) from the layer is calculated from SW(L), DUL(L), DLAYR(L), and SWCON, the whole profile drainage rate constant.

DRAIN = (SW(L) - DUL(L)) \* SWCON \* DLAYR(L).

At this point, a drained value of SW(L) is calculated,

SW(L) = SW(L) - DRAIN/DLAYR(L),

and a new value of FLUX(L), representing water moving into the layer below, is set equal to DRAIN.

If FLUX(L) is greater than HOLD, the water in excess of HOLD is passed directly to the layer below by saturated flow. The drainage is then calculated as follows:

DRAIN = SWCON \* (SAT(L) - DUL(L)) \* DLAYR(L).

An updated value for FLUX(L) is calculated

FLUX(L) = FLUX(L) - HOLD + DRAIN.

After calculating the water movement through all soil layers, any drainage from the bottom layer of the profile is equal to FLUX(L). For convenience, this value is converted to mm by multiplying by 10, and set equal to DRAIN. DRAIN then represents the total outflow from the lowest layer of the soil profile and is an available output variable for those interested in the time course of drainage out of the soil profile

## EVAPOTRANSPIRATION

The soil water balance subroutine requires calculations for potential evaporation from the soil and plant surfaces.  The equations to predict evaporation are primarily those used in the model of Ritchie (1972). The main difference between this part of the soil water balance subroutine and the Ritchie model is that a Priestly-Taylor (1972) equation for potential evapotranspiration is used instead of the Penman equation. This was done to eliminate the need for vapor pressure and wind inputs and under many circumstances it provides equal accuracy.

Calculation of potential evaporation requires an approximation of daytime temperature (TD) and the soil-plant reflection coefficient (ALBEDO) for solar radiation. For the approximation of the daytime temperature a weighted mean of the daily maximum (TEMPMX) and minimum (TEMPMN) air temperatures is used:

TD = 0.6 \* TEMPMX + 0.4 \* TEMPMN.

The combined crop and soil albedo (ALBEDO) is calculated from the model calculated leaf area index (LAI) and the input bare soil albedo (SALB). Prior to germination, ALBEDO is equal to SALB. For Stages 1 to 4 the value for ALBEDO is

ALBEDO = 0.23 - (0.23 - SALB) \* EXP(-0.75 \* LAI).

For stages 4 to 6, ALBEDO is

ALBEDO = 0.23 + (LAI - 4) \*\* 2 / 160.

An equilibrium evaporation rate (EEQ) defined in Priestly and Taylor (1972) is calculated from ALBEDO, TD, and the input solar radiation SOLRAD.

EEQ = SOLRAD \* (4.88 \* 10-3 - 4.37 \*10-3 \* ALBEDO) \* (TD + 29),

(Fig. 3.2). The units of EEQ is mm day-1 and SOLARD is MJ m-2 day-1. This empirical equation is a simplification of one containing long wave radiation approximations needed to calculate net radiation.

Fig. 3.2. EEQ/SOLARD versus TD.

The potential evaporation (EO) is calculated as the product of EEQ times 1.1. The constant 1.1 increases EEQ to a larger value to account for unsaturated air. This assumption is from the Priestley-Taylor assumption that the aerodynamic component of evaporation is proportional to the radiant energy into the system. The combustion equation assumes that the two terms are additive. When TEMPMX is greater than 24 C, the constant 1.1 is increased to account for advection

EO = EEQ \* ((TEMPMX - 24) \* 0.05 + 1.1).

When TEMPMX is less than 5 C, the constant is reduced to account for cold temperature causing an additional decrease in EO due to stomata closure.

EO = EEQ \* 0.01 \* EXP(0.18 \* (TEMPMX + 20)).

Fig. 3.3 graphically demonstrates how TEMPMX affects this constant multiplier for EEQ.

Fig. 3.3. TEMPMX relationships.

The potential rate of soil evaporation (EOS) is then calculated using the leaf area index, LAI. When LAI is less than 1,

EOS = EO \* (1 - 0.43 \* LAI),

and when LAI is greater than 1,

EOS = EEQ \* EXP(-0.4 \* LAI).

The calculation for the actual rate of soil evaporation (ES) is based on the assumption that there are two stages of soil evaporation. The first stage is limited by the energy available at the soil surface and continues until a soil-dependent upper limit is reached. This upper limit for stage 1 evaporation is expressed by the input U. After the upper limit of stage 1 is reached, soil evaporation enters stage 2. In stage 2, the rate of evaporation decreases proportionally to the time spent in stage 2.

The variables SUMES1 and SUMES2 are the sums of the soil evaporation (ES) in stages 1 and 2, respectively, and are used to determine which stage of soil evaporation is occurring during a day.

When rainfall or irrigation occurs during a day, and the infiltration into the upper layer is greater than or equal to SUMES1, SUMES1 is set back to 0. If, however, WINF is less than SUMES1, then SUMES1 is updated by the following equation:

SUMES1 = SUMES1 - WINF.

Whenever SUMES1 is less than the upper limit of stage 1 evaporation (U), SUMES1 is updated daily by the following:

SUMES1 = SUMES1 + EOS.

If the new value of SUMES1 is less than or equal to U, then

ES = EOS.

If, however, the new value of SUMES1 is greater than U, then

ES = EOS - 0.4 \* (SUMES1 - U),

using the new value of SUMES1.

Should the value for SUMES1 exceed U, the soil evaporation enters stage 2, and SUMES2 is calculated.

SUMES2 = 0.6 \* (SUMES1 - U).

The time after the beginning of stage 2 evaporation (T) is then calculated.

T = (SUMES2/3.5)\*\*2.

As the soil continues to dry during stage 2 evaporation, the value for T increases by 1 daily. The value for soil evaporation (ES) is calculated as follows:

ES = 3.5 \* T\*\*0.5 - SUMES2.

When ES calculated in this manner is less the EOS, the value for ES is set to equal EOS.

When rainfall or irrigation occur during stage 2 evaporation and only slightly wet the soil, if WINF is less than SUMES2, then ES is set equal to the minimum of EOS, 0.8 \* WINF, or ES + WINF.

During stage 2 evaporation, SUMES2 and T are updated daily.

SUMES2 = SUMES2 + ES - WINF.

T = (SUMES2/3.5)\*\*2.

If during Stage 2 evaporation, rainfall and/or irrigation wet the soil surface slightly more than described above such that WINF is greater than SUMES2, the value for T is reset to 0 and SUMES1 is calculated.

SUMES1 = U - WINF + SUMES2.

When this has occurred, the soil evaporation has re-entered Stage 1 and Stage 1 evaporation is calculated as described earlier.

After ES has been determined, the water is subtracted from the volumetric water content of soil layer 1 (SW(1)). If SW(1) decreases such that its value is less than SWEF \* LL(1), ES is recalculated so that SW(1) does not become less than SWEF \* LL(1). The term SWEF is considered the driest possible soil water content and is used to limit the drying of the soil by evaporation to a reasonable limit. The value of SWEF is approximately half the value of LL(1), with some variation depending on the layer thickness (DLAYR(1)).

The upward flow of water in the top 4 soil layers is next calculated to account for the movement of water, which usually moves toward the soil surface during evaporation. This upward flow is principally needed in the nitrogen subroutines to account for upward movement of nitrogen.

The variables THET1 and THET2 represent a normalized volumetric water content of layers L and L + 1, respectively as follows:

THET1 = SW(L) - LL(L),and

THET2 = SW(L + 1) - LL(L + 1),

and values of THET1 and THET2 are constrained to be no less than 0. Thus the water content is normalized to the lower limit (LL(L) where the assumption is made that the diffusivity for all soils is similar. The assumed diffusivity (DBAR) is a function of the normalized water content for all soils

DBAR = 0.88\*EXP(35.4 \* (THET1 \* 0.5 + THET2 \* 0.5)),

where DBAR is not allowed to be greater than 100. The unit of DBAR is cm day-1/2. The flow of water is then calculated:

FLOW = DBAR \* (THET2 - THET1)/((DLAYR(L) + DLAYR(L + 1)) \* 0.5).

A plot of DBAR, the soil water diffusivity, is shown in Fig. 3.4. The volumetric soil water in layers L and L + 1 are then increased and decreased by the amount of FLOW, and the new volumetric soil water is calculated.

SW(L) = SW(L) + FLOW/DLAYR(L),

SW(L + 1) = SW(L + 1) - FLOW/DLAYR(L + 1).

Fig. 3.4. Soil water diffusivity.

For user information the cumulative soil evaporation after germination (CES) is updated daily,

CES = CES + ES,

The potential plant evaporation (EP) is calculated using simulated LAI values less than or equal to 3.

EP = EO \* LAI/3,

When LAI is greater than 3,

EP = EO.

If EP + ES is greater than EO, then

EP = EO - ES.

Reducing EP from a potential value to an actual one requires the calculation of root water absorption.

## ROOT WATER ABSORPTION

The root water absorption in CERES-Wheat is calculated using a law of the limiting approach whereby the soil resistance, the root resistance, or the atmospheric demand dominate the flow rate of water into the roots. Most of the details of this approach have been discussed by Ritchie (1984). The flow rates are calculated on the basis of water movement to a single root.

The maximum daily water uptake by roots in a layer (RWUMX) is assumed to be 0.03 cm3 of water per cm of root. This value sets the upper limit of water absorption by the roots as limited by axial root resistance. The potential root water uptake as influenced by soil water flow in a layer (RWU(L)) is

RWU(L) = 0.00267 \* EXP(62 \* (SW(L) - LL(L)))/(6.68 - ALOG(RLV(L))),

where RLV(L) is the root length density in the soil layer and ALOG is the FORTRAN equivalent of natural logarithm. This equation was derived from a radial flow to a single root and assumes that the hydraulic conductivity of all soils are similar when normalized to the lower limit value, LL(L). This assumption is more generally correct when the soil water content is near the lower limit. This equation also assumes that the water potential gradient between the root and the soil remains constant, even when the soil dries out. In reality, the water potential of the roots changes considerably throughout the day. However, because we are calculating daily values for water absorption, these less dynamic empiricisms provide sufficient detail for realistic uptake simulations.

If the calculated value for RWU(L) is greater than RWUMX, then RWU(L) is set equal to RWUMX (Fig. 3.5). The units of RWU(L) are then changed from cm3/cm of root to cm of water in a soil layer by the following:

RWU(L) = RWU(L) \* DLAYR(L) \* RLV(L),

and the total potential root water uptake from the entire root zone (TRWU) is calculated as the sum of RWU(L) for all soil layers with roots.

Fig. 3.5. The relationship used to calculate maximum root water absorption as related to O-' (the water content above the lower limit) and root length density (Lv). Also shown is the assumed maximum possible rate and the usual range of absorption when all the soil profile is at an optimum water content.

The terms TRWU and RWU(L) are potential water uptake values and represent the maximum possible water uptake from the soil profile and a root layer, respectively. A water uptake fraction (WUF) is calculated to reduce the potential root water uptake to the actual if necessary.

WUF = EP1/TRWU

where EP1 is the potential transpiration in cm day-1. If WUF is less than or equal to 1.0, the plants are considered to be free of a water deficit so that the potential EP value is obtained. If WUF is greater than 1, then the actual plant evaporation is equal to the sum of the root absorption rates. Actual water uptake in each layer, RWU(L), is then calculated for the case when WUF is less than or equal to 1.0

RWU(L) = RWU(L) \* WUF.

Values of SW(L) are updated,

SW(L) = SW(L) - RWU(L)/DLAYR(L),

and the total soil water in the profile (TSW) is calculated:

TSW = TSW + SW(L) \* DLAYR(L).

The potentially extractable soil water in the entire soil profile (PESW) can now be calculated from TSW minus the total water content of the profile at the lower limit of the plant-extractable soil water (TLL):

PESW = TSW - TLL,

The soil water deficits SWDF1 and SWDF2, used in the growth routine of CERES-Wheat, are now calculated:

SWDF1 = TRWU/EP1

SWDF2 = 0.67 \* TRWU/EP1,

SWDF1 and SWDF2 are constrained to be no greater than 1.0 (Fig. 3.6). If SWDF1 is not less than 1, the plant evaporation (EP) is assumed to be equal to the potential EP. If SWDF1 is less than 1, then the actual is equal to the maximum absorption rate (TRWU).

EP = TRWU \* 10.

The 10. converts the units of EP to mm day-1. Actual daily value of soil plus plant evaporation now becomes

ET = ES + EP.

Fig. 3.6. Relationship used to calculate soil water factors, SWDF1 and SWDF2, to incorporate water stresses in the model.

To summarize the information on the soil water deficit influence on plants, two values are calculated:  CSD1 and CSD2.  These values are an average of the SWDF1 and SWDF2 during each growth stage.  The values are not used in the model, but are given to provide information to the user for possible interpretation of the yield responses related to soil water deficits.  The values appear on the printouts of the output summary sheet.

## COLD HARDENING

Hardening, is a biochemical change that permits plants to survive under colder temperatures without being killed.  Hardening occurs in the -0`C range (0 to -5`C or -10`C).  These temperatures are not cold enough to kill the plants, but they are below the base temperature for them to be able to function.  The longer a plant is in this state, the hardier it becomes and the longer it can withstand cold temperatures.

Plants go through two stages of hardening.  The first stage is described above.  The second stage occurs with even colder temperatures.  A plant then can withstand the worst of conditions, though it can still be killed.  (An unhardened plant will be killed by much higher temperatures than a hardened plant.)

The cold hardiness calculation in the CERES-Wheat model uses a hardiness index (HI) whose value varies between 0 and 2.  Plants with HI values between 0 and 1 are considered to be in stage 1 hardening.  Plants with HI values between 1 and 2 are in stage 2 hardening.

There are some limitations of this model for cold hardiness.  It does not account for cold-sensitive wheat varieties planted where winter temperatures can kill the plants (we assumed only cold-resistant varieties would be planted in these areas).  Genetic differences are not considered, as sufficient quantitative evidence to develop the necessary relationship for such differences is lacking.  Also, this part of the model was not tested very thoroughly because we lacked the quantitative information from field experiments.

In the model, the vernalization process is started after the seed has germinated, because the activated seed can go through vernalization.  In stage 9 and 1, the model automatically calls the cold subroutine.  Hardening occurs from -1`C and -8`C.  The quantitative expression in the model for the hardiness index is

HI = HI + 0.1 - (TEMPCR - (TBASE + 3.5)) \*\* 2/506

where HI is the hardiness index and TEMPCR is the temperature at the crown.  The HI is updated daily using this expression; HI in the left side of the equation comes from the previous day, and HI in the right side is the new HI.  The expression is valid only between -1`C and 8`C.  If the HI is 3.5, it would take 10 days for the HI to equal 1.  Therefore, 10 days is the minimum time for a plant complete stage 1.

Stage 2 hardening is calculated when the first stage is greater than 1 and is then updated daily.  (All plants must go through stage 1 before starting stage 2.)  Any day the crown temperature is less than 0, the model takes the old value and adds 0.083 per day:

HI = HI + 0.083.

Under these conditions the plant will harden and HI will be at 2--maximum hardness--in 12 days.

Critical for the dehardening process is the maximum temperature (TEMPMX).  Dehardening does not occur if TEMPMX is less than 10`C (Gusta and Flower 1976).  If TEMPMX is 10, at 20`C, it loses 0.2 HI,

HI = HI + 0.2 - 0.02 \* TEMPMX.

If the plant is in stage 2 hardening, the rate of daily dehardening is doubled.

After cold hardiness, leaf senescence is calculated if the minimum temperature is below -6`C.  If these conditions exist, the model calculates the fraction of green leaf area (CR) killed using the expression

CK = (0.20 \* HI - 0.10) \* (TEMPMN \* 0.85 + TEMPMX \*

0.15 + 10 + 2.5 \* SNOW

where SNOW is the snow depth in centimeters.  The expression, empirically derived, accounts for slight modifications in senescence due to hardening and a strong influence related to the protection of the snow.  Once CK is calculated the senescent leaf area (SENLA) is updated:

SENLA = SENLA + CK \* (PLA - SENLA)

where PLA is the total plant leaf area developed during the plant's life.

If the plants have not been killed by the cold temperatures, a logical statement in the program prevents the green leaf area of each tiller from being less than 0.5 sq.cm.  If the leaves and roots are senesced to that minimum point (0.5), the crown is assumed to contain 0.5 g of reserve carbohydrates for use in regrowth in much the same way.  The stored carbohydrate is treated in the same way as the seed reserve was in helping to establish a new seedling before the plant becomes capable of independently producing enough assimilate for independent growth.

The next calculation is the death of tillers and plants.  The threshold killing temperature (TEMKIL) for any death is calculated from the expression

TEMKIL = TBASE - 6 - 6 \* HI.

This calculation shows that hardening has a lot to do with how much a plant will be killed by cold temperatures.  TEMKIL is the threshold temperature by which plants begin to be killed.  If a crown temperature is below that threshold, killing occurs by a reduction in tiller number if there is more than one tiller per plant.  The expression for killing tillers is

TILN = TILN \* (0.9 - 0.02 \* (TEMPCR - TEMKIL) \*\* 2).

If all but one tiller are killed, the plant population must be reduced.  The reduction is done with an expression similar to tiller death:

PLANTS = PLANTS \* (0.95 - 0.02 \* (TEMPCR - TEMKIL) \*\* 2).

If the plant population is reduced to less than five plants per square meter, the plant growth parts of the program are terminated and a message is printed stating that the crop has failed due to cold temperatures. To help users interpret possible reasons for yield reduction, a message is also written for days that the crop is damaged by cold temperatures.

# CHAPTER 4

# NITROGEN COMPONENTS

## DESCRIPTION OF THE MODEL AND APPROACHES TO MODELING N DYNAMICS

The nitrogen dynamics routines of the CERES models were designed to simulate each of the major N loss processes and the contributions to the N balance made by mineralization. The routines also describe the uptake of N by the crop and the effects of N deficiency on crop growth processes. The transformations simulated are mineralization and/or immobilization, nitrification, denitrification, and urea hydrolysis. Nitrate movement associated with water movement in both an upward and downward direction is also simulated. Since the rates of transformation of nitrogen are very much influenced by soil water status, the simulation of nitrogen dynamics requires that water balance also be simulated. Soil temperature greatly influences many of the transformation rates. Therefore, a procedure to calculate soil temperature at various depths, based on the soil temperature routine of the EPIC model (Williams et al. 1984), is also invoked in the nitrogen component of the model.

The model does not simulate losses by ammonia volatilization or ammonium exchange equilibria and fixation. Under conditions of good fertilizer practice where fertilizer is either incorporated or placed beneath the soil surface, volatile ammonia losses should be small.

## INITIALIZATION

Inputs describing the amount of organic matter and the amount of mineral nitrogen present in the soil are required to initialize the model. The model requires the organic carbon concentration in each layer (OC(L)) as an input and using an assumed soil C:N ratio of 10:1 calculates the amount of organic N associated with this organic matter (HUM(L)). These initializations are performed in subroutine SOILNI. To determine the contribution of recent crop residues to the supply of nitrogen in the soil, the model also requires an estimate of the amount of crop residue (STRAW) which is present. Based on this estimate and the depth of incorporation (SDEP) of the crop residue, the fresh organic matter content of each layer (FOM(L)) is estimated. An estimate of the amount of root residue remaining from the previous crop is also required for the calculation of FOM(L). Procedures for estimating STRAW and ROOT and the default values used are described in Chapter 6. Initial partitioning of the fresh organic matter into the component pools of carbohydrate (FPOOL(L,1)), cellulose (FPOOL(L,2)) and lignin (FPOOL(L,3)) is also performed in subroutine SOILNI.

## NITRATE FLUX

Leaching of nitrates is probably the most common and best understood N loss process. Nitrates leaching from soil often become a source of contamination of groundwater and has recently generated interest in leaching from an environmental standpoint. There have been many approaches to modelling leaching based on numerical techniques which require solution in a manner inappropriate for use in a management level model such as CERES. In the CERES model, leaching is simulated using a simple approach based on the cascading system for drainage described in the previous chapter. Nitrate N may move between layers of the soil profile in the CERES models, 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. Therefore, 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 0.25 g NO3 per g of soil 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 the 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 the soil 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 movement (FLOW(L)) in a manner identical to leaching:

NUP = SNO3(L) \* FLOW(L)/(SW(L) \* DLAYR(L) + FLOW(L)) \* 0.5

No upward 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 is set up with calculations commencing in the top layer and running to lower layers. This is achieved by first reinitializing the array FLUX to 0 and reversing the sign (to make it positive) at the FLOW array and copying it to FLUX. When this has been done the normal leaching calculations used in the first loop can be used again. These instances would occur when a small rainfall wets the top layer of a very dry soil profile. There may have been insufficient water for drainage to occur but a moisture potential between the top layer and the second layer initiates this flow. The resultant movement of nitrate will be very small.

## 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.

**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. In addition to the numeric code for fertilizer type, inputs required to describe the fertilizer are: the date of application (FDAY), 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. These must correspond with those used to describe the soil water inputs. Surface fertilizer applications are treated as being uniformly incorporated into the top layer. Up to 10 split applications can be accommodated by the model.

**Mineralization and Immobilization**

Mineralization refers to the net release of mineral nitrogen with the decay of organic matter and immobilization refers to the transformation of mineral nitrogen to the organic state. Both processes are microbial in origin. 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 can often constitute a large part of the nitrogen available to the crop.

The perceived application for the CERES models in studies examining crop growth and fertilizer management requires that a mineralization model be simple, require few inputs, and work on a diversity of soils. Simulation studies examining the affects of crop residues also requires that the model be capable of simulating the fate of residues of different compositions. Other studies examining the potential role of nitrification inhibitors 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 microbiological level models but doing so at a very simplified level. The model's modifications have been to simulate nitrification separately and to partition the simulated fresh organic matter pools differently. Modifications were also made to temperature and water indices to fit the CERES water balance and soil temperature routines. Unless otherwise indicated, the coefficients used for the mineralization/immobilization functions described below were drawn from the PAPRAN model.

The mineralization and immobilization routine simulates the decay of two types of organic matter: 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 is selected according to the proportion of the initial amount of FOM remaining. The CERES model separates FOM into three pools giving 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) and an estimate of the amount of root residue from the previous crop. Based upon these data, initial values of FOM and the N contained within it (FON) for each layer are calculated in subroutine SOILNI. The soil organic carbon in each layer (OC(L)) is also required by the mineralization routine. 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 carbohydrate, cellulose, and lignin, respectively. A decay constant at 0.20 for the carbohydrate fraction has since been found to be more appropriate. The decay constant for carbohydrate implies that under nonlimiting conditions 20% 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), and drained upper limit (DUL). In accordance with the soil water balance model, provision is made for the water content of the uppermost layer to be lower than the lower limit. The variable SWEF determines the lowest possible value the uppermost soil layer water content have. When the soil is drier than DUL, MF is calculated as:

AD = LL(L)

IF (L.EQ.1) AD = LL(1) \*SWEF

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

where:

AD = lowest moisture content for a layer (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) on moisture effects on ammonification. 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, 1984). The comparative effects of soil moisture on the simulated rates of ammonification, nitrification, and denitrification can be seen in Fig. 5.1. A temperature factor (TF) is calculated directly from soil temperature (ST(L)):

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

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 5o 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)

Thus, 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 (Fig. 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. 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,GRCOM\*(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.

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 a sufficient amount to retain this pool with a concentration of 0.5 ppm, withdrawals are made from the nitrate pool.

**Nitrification**

Nitrification refers to the process of oxidation of ammonium to nitrate. It is a biological process and occurs under aerobic conditions. The main factors which limit nitrification are: Substrate NH4+, oxygen, soil pH, and temperature. 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 was 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 reported 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. First, 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) (Fig. 3.4) are used together with SANC to determine an environmental limit on nitrification capacity (ELNC).

ELNC=AMIN1(TF,WFD,SANC)

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 an index for pH effect on nitrification. This pH index is calculated in subroutine SOILNI and represents the conclusions drawn by Schmidt (1982) on the pH effect in nitrification.

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 maximum of 80% at the ammonium pool is allowed to nitrify in one day. 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 the nitrification calculations 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.

**Denitrification**

Denitrification is the dissimilatory reduction of nitrate (or nitrite) to gaseous products including N0, N20, and N2 (Knowles, 1981).

Denitrification is a microbial process which occurs under anaerobic conditions and is influenced by organic carbon content, soil aeration, temperature and soil pH. 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 favorably 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 Fig. 5.1) 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 (1983) used percentage of water filled porosity as an index of soil water availability effects on soil N transformations. In their studies, 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. 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. (1971) to 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 = FAC(L)\*(SOILC\*0.0031+0.4\*FPOOL(L,1))+24.5

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)

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

## 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 additional inputs 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. 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 more shallow than this, diurnal change in temperature occurs with the greatest fluctuation happening near 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) \* (TEMPM + (TEMPMX - TEMPM) \*

SQRT(SOLRAD \* 0.03)) + 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 MJ/square metre.

TEMPMX,TEMPM = 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 2 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.

## PLANT CRITICAL N CONCENTRATIONS AND N DEFICIT FACTORS

Plant growth is greatly affected by the supply of N. Typically the supply of N to plants at the beginning of the season is often relatively high and becomes lower as the plant reaches maturity. The concentration of N in plant tissues also changes as the plant ages. During early growth, N concentrations are usually high due to synthesis of large amounts of organic N compounds required by the biochemical processes constituting photosynthesis and growth. As the plant ages, less of this new material is required and export from old tissues to new tissues occurs lowering the whole plant N concentration. At any point in time there exists a critical N concentration in the plant tissue below which growth will be reduced. 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 model's critical concentration functions 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 a fractional growth stage which is used to determine an approximate value for the corresponding Zadoks' stage (ZSTAGE). The conversions were performed using several functions which are tabulated below (Table 1). The functions are located in subroutine NFACTO.

Table 1. 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)

To develop appropriate relationships for critical N concentrations in wheat, published data from field experiments that met the following criteria were assembled:

1. Experiments had a series of N rates with sufficient range to define optimal or near-optimal growth patterns.

2. Experiments were considered to have been conducted under conditions where the potential effects of other interacting factors (e.g., heat stress, moisture stress, frost, supply of other nutrients, etc.) were minimized.

3. Plant tops N concentration was reported at several times during the growing season.

4. The growth stage or phenological age of the crop was reported for the times of plant sampling.

In some cases, critical concentrations were defined by the authors and where appropriate were adopted. In two studies only one N rate was used but was described as being an optimal rate by the authors. Data were drawn from the following sources (Table 2) representing a diversity of wheat genotypes and wheat-growing environments.

Table 2. Data Sources Used for Determination of Critical N Concentration Relationships

Author Spring or Winter Wheat Location

Engel and Zubriski (1982) Spring North Dakota

Campbell et al. (1977a) Spring Canada

Wagger et al. (1981) Winter Kansas

Leitch and Vaidanathan (1983) Winter U.K.

Wagger (1983) Winter Kansas

Waldren and Flowerday (1979) Winter Nebraska (?)

Page et al. (1977) Winter U.K.

Alessi et al. (1979) Spring North Dakota

Mugwira and Bishnoi (1980) Winter Alabama

Boatwright and Haas (1961) Spring North Dakota

Gasser and Thorburn (1972) Spring U.K.

Bhargava and Motiramani (1967) Spring Australia

Walia et al. (1980) Spring India

McNeal et al. (1968) Spring Montana

Spratt and Gasser (1970) Spring U.K.

From these data, relationships defining critical N concentration as a function of Zadoks' growth stage were determined. The critical N concentration was defined as the N concentration in the plant tissues at optimal or near optimal growth (as defined by biomass, yield or leaf area from the response data). The relationship thus determined is defined as the concentration above which no further increases in crop growth occur and below which some effect on a growth process will occur. Winter wheats and spring wheats were found to have different relationships (Fig. 3.7). The differences between winter and sprin wheats may be an artifact created by the different growing conditions of the experiments cited above. It has been difficult to characterize critical concentrations particularly for the period of rapid growth in the spring when phenological age, N uptake and biomass are all increasing rapidly. These relationships for the tops critical N percentage TCNP) appear in subroutine NFACTO as a function of Zadoks' growth stage (ZSTAGE).

For winter wheats:

TCNP = -5.0112 - 6.3507 \* ZSTAGE + 14.9578 \* SQRT(ZSTAGE) +

0.2238 \* (ZSTAGE \* ZSTAGE)

For spring wheats:

TCNP = 7.4532 - 1.7908 \* ZSTAGE + 0.6093 \* SQRT(ZSTAGE) +

0.0934 \* ZSTAGE \* ZSTAGE

Root critical N concentration (RCNP) relationships were derived from the greenhouse data of Peterson et al. (1983) and Day et al. (1985).

RCNP = 2.10 - 0.14 \* SQRT(ZSTAGE)

The minimum concentration of N in plant tissues as a function of plant age is seldom reported. To formulate an appropriate relationship for use in the model, some of the minimum concentrations reported in the above studies were used as well as those reported from an extensive survey of N concentration in wheat crops spanning several years and locations in South Australia by Schultz and French (1976). In the model the tops minimum concentration (TMNC) is calculated as a function of model growth stage (XSTAGE):

TMNC = 2.97 - 0.455 \* XSTAGE

Root critical minimum N concentration (RMNC) is used during the grain filling calculations (in subroutine GROSUB) and is assumed to be a constant 75% of the critical concentration.

RMNC = 0.75 \* RCNP

The coupling of these functions to the phenology routines thus enables critical concentrations to be determined for any variety growing in any environment. The critical and minimum concentrations are used to define a nitrogen factor (NFAC) which ranges from zero to slightly above unity. NFAC is the primary mechanism used within the model to determine the effect of N on plant growth. It is an index of deficiency relating the actual concentration (TANC) to these critical concentrations. NFAC has a value of zero when TANC is at its minimum value of TMNC and increases to 1.0 as concentration increases toward the critical concentration. NFAC is calculated as:

NFAC = 1.0 - (TCNP - TANC)/(TCNP - TMNC)

Since all plant growth processes are not equally affected by N stress, a series of indices based on NFAC are used. For photosynthetic rate (NDEF1) the index is calculated as:

NDEF1 = 0.10 + 2.0 \*NFAC (NDEF<1.0)

For leaf expansion growth (NDEF2) a more sensitive factor is used:

NDEF2 = NFAC

For tillering (NDEF3) the index is calculated as:

NDEF3=NFAC\*NFAC

For the calculation of these indices NFAC has a maximum value of 1.0. This implies that when TANC exceeds TCNP no extra growth occurs. A fourth factor used to modify the rate of grain N accumulation (NDEF4) is also calculated from NFAC, and can range from 0.0 to 1.5.

NDEF4 = NFAC \* NFAC

These relations are depicted in Fig. 3.8. In the growth subroutine, GROSUB, the law of the minimum is used extensively to modify rates of plant growth. For each of the major functions (e.g., photosynthetic rate, leaf expansion rate, tiller number determination) the minimum of several zero to unit stress indices is used to modify a potential rate for the process.

## N UPTAKE

The approach used in the CERES models has been to separately calculate the components of demand and supply and then use the lesser of these two to determine the actual rate of uptake. Demand can be considered as having two components. First there is a "deficiency demand." This is the amount of N required to restore the actual N concentration in the plant (TANC for tops) to the critical concentration (TCNP for tops). Critical concentrations for shoots and roots are defined in section 3.7. This deficiency demand can be quantified as the product of the existing biomass and the concentration difference as below:

TNDEM = TOPWT \* (TCNP - TANC)

Similarly for roots the discrepancy in concentration (difference between RCNP and RANC) is multiplied by the root biomass (RTWT) to calculate the root N demand.

RNDEM = RTWT \* (RCNP-RANC)

If luxury consumption of N has occurred such that TANC is greater than TCNP then these demand components have negative values. If total N demand is negative then no uptake is performed on that day. The second component of N demand is the demand for N by the new growth. Here the assumption is made that the plant would attempt to maintain a critical N concentration in the newly formed tissues. To calculate the new growth demand, a potential amount of new growth is first estimated in the GROSUB subroutine. New growth is estimated from potential photosynthesis (PCARB) and is partitioned into a potential root growth (PGRORT) and a potential tops growth (PDWI). Partitioning between potential shoot and root growth occurs as a function of phenological age:

PGRORT = PCARB \* (60 - XSTAGE \* 8)/100

PDWI = PCARB - PGRORT

These potential growth increments provide a mechanism for the tops actual N concentration (TANC) to exceed TCNP. This occurs when some stress prevails and the actual growth increment is less than the potential. New growth demand for tops (DNG) is calculated as

DNG = PDWI \* TCNP

and the new growth demand for roots is calculated as

PGRORT \* RCNP.

During the early stages of plant growth the new growth component of N

demand will be a large proportion of the total demand. As the crop biomass increases the deficiency demand becomes the larger component. During grain filling, the N required by the grain is removed from the vegetative and root pools to form a grain N pool. The resultant lowering of concentration in these pools may lead to increased demand. The total plant N demand (NDEM) is the sum of all of these demand components. Calculations of soil supply of N are on a per hectare basis which necessitates recalculation of the per plant demand into a per hectare demand (ANDEM).

ANDEM = NDEM \* PLANTS \* 10.0

To calculate the potential supply of N to the crop, zero to unity availability factors for each of nitrate (FNO3) and ammonium (FNH4) are calculated from the soil concentrations of the respective ions:

FNO3 = 1.0 - EXP(-0.0275 \* NO3(L))

FNH4 = 1.0 - EXP(-0.025 \* NH4(L))

The coefficients used in these two functions, obtained by trial and error, were found to be appropriate over a range of data sets. The greater mobility of nitrate ions in soil is reflected by the larger coefficient (0.0275) in these equations. A zero to unity soil water factor (SMDFR) which reduces potential uptake is calculated as a function of the relative availability of soil water:

SMDFR = (SW(L) - LL(L)/ESW(L)

To account for increased anaerobiosis and declining root function at moisture contents above the drained upper limit, SMDFR is reduced as

saturation is approached.

IF(SW(L) . GT . DUL(L))SMDFR = 1.0 - (SW(L) - DUL(L))/(SAT(L) - DUL(L))

The maximum potential N uptake from a layer may be calculated as a function of the maximum uptake per unit length of root and the total amount of root present in the layer. The first of these is a temporary variable (RFAC) which integrates the effects of root length density (RLV(L)), the soil water factor described above, and the depth of the layer:

RFAC = RLV(L) \* SMDFR \* SMDRF \* DLAYR(L) \* 100.0

The second of these equations incorporates the ion concentration effect (FNO3) and the maximum uptake per unit length of root (0.009 kg N/ha cm root) to yield a potential uptake of nitrate from the layer (RNO3U(L)).

RNO3U(L) = RFAC \* FNO3 \* 0.009

(RNO3U(L)) is thus the potential uptake of nitrate from layer L in kg N/ha constrained by the availability of water, the root length density and the concentration of nitrate. Initial estimates for the maximum uptake per unit length of root coefficient were obtained from the maize root data of Warncke and Barber (1974). This estimate was the subject of continuing modification during early model development. The value reported here appears to be appropriate across a broad range of data sets. The effect of each of these parameters on determining potential uptake can be seen in Fig. 3.9. A similar function is employed to calculate the potential uptake of ammonium (RNH4U(L)).

RNH4U(L) = RFAC \* FNH4 \* 0.009

Potential N uptake from the whole profile (TRNU) is the sum of RNO3U(L) and RNH4U(L) from all soil layers where roots occur. Thus TRNU represents an integrated value which is sensitive to (a) rooting density, (b) the concentration of the two ionic species, and (c) their ease of extraction as a function of the soil water status of the different layers. This method of determining potential uptake enables the common condition, where N is concentrated in the upper layers of the profile, where most of the roots are present and where a nutritional drought due to shortage of water in these upper layers may occur, to be simulated. This can occur when the crops demand for water is satisfied from soil water located deeper in the profile but where there may be little N present. If the potential N supply from the whole profile (TRNU) is greater than the crop N demand (ANDEM) an N uptake factor (NUF) is calculated and used to reduce the N uptake from each layer to the level of demand.

NUF = ANDEM/TRNU

This could occur when plants are young and have a high N supply. If the demand is greater than the supply then NUF has a value of 1.0. When NUF is less than 1.0, uptake from each layer is reduced as follows:

UNO3 = RNO3U(L) \* NUF

UNH4 = RNH4U(L) \* NUF

Following these calculations the soil mineral N pools can be updated for the actual uptake which has occurred.

SNO3(L) = SNO3(L) - UNO3

SNH4(L) = SNH4(L) - UNH4

Under conditions of luxury N uptake (TANC > TCNP) exudation of organic N compounds can occur. Rovira (1969) found changes in the shoot environment which cause more rapid growth can increase exudation. Bowen (1969) reported that N deficiency can cause exudation to decrease. In the CERES-N model this exuded N is added to the fresh organic N pool (FON(L)) and can be mineralized and subsequently made available to the plant again. The amount of N which can be lost from the plant in this manner is calculated as 5% of the N contained in the roots/day. These losses are distributed to the FON(L)) pool according to the differing root length densities present in each layer as a proportion of the total root length.

IF(TANC . GT . TCNP)RNLOSS = RANC \* RTWT \* 0.05 \* PLANTS \* RLV(L)/TRLV

Following uptake, concentrations of N in each of the shoots and roots are updated. To do this TRNU is converted from kg N/ha to a g N/plant basis.

TRNU = TRNU/(PLANTS \* 10.0)

The proportion of the total plant demand (NDEM) arising from shoots (TNDEM) and roots (RNDEM) and the total root N loss (TRNLOS) are used to calculate the changes in N content of the shoots (DTOPSN) and roots (DROOTN).

DTOPSN = TNDEM/NDEM \* TRNU - PTF \* TRNLOS/(PLANTS \* 10.0)

DROOTN = RNDEM/NDEM \* TRNU - (1.0 - PTF) \* TRNLOS/(PLANTS \* 10.0)

TRNLOS is distributed over shoots and roots according to the plant top fraction (PTF) and must also be converted from a unit area basis to a per plant basis. Shoot and root N pools (TOPSN and ROOTN, respectively) can then be updated and new concentrations calculated:

TOPSN = TOPSN + DTOPSN

ROOTN = ROOTN + DROOTN

TANC = TOPSN/TOPWT

RANC = ROOTN/(RTWT - 0.01 \* RTWT)

When updating the root concentration allowance is made for the losses in root biomass occurring due to root exudation.

## N REDISTRIBUTION DURING GRAIN GROWTH AND GRAIN N DETERMINATION

In many wheat-growing areas when the crop reaches the grain-filling stage soil supplies of N are very low. In these cases the nitrogen requirement of the developing grains is largely satisfied by remobilization of protein from vegetative organs. When nitrogen supply is increased, the proportion of grain N arising from remobilization declines, and the proportion from uptake increases (Vos 1981). Many studies (e.g., Benzian et al., 1983, Terman et al., 1969) have found negative correlations between grain yield and grain protein concentration. Temperature and soil moisture also affect the grain nitrogen content. When constructing the N grain-filling routines, procedures were adopted to closely mimick those predicting grain mass (or carbon) accumulation. In this procedure the rate of grain filling (RGFILL) (mg/day) is determined by temperature and thermal time (DTT).

To define similar functions for the rate of grain N accumulation (RGNFIL) (in micrograms per kernel per degree C day), the controlled environment studies of Sofield et al. (1977), Vos (1981) and Bhullar and Jenner (1985) were used. These studies examined various cultivars over a range of temperature conditions and other treatments. The relationship which best described these studies and mimicked the grain mass accumulation functions was:

RGNFIL = 4.8297 - 3.2488 \* DTT + 0.2503 \*(TEMPMX - TEMPMN) +

4.3067 \* TEMPM

and when the mean temperature is less than 10

RGNFIL = 0.483 \* TEMPM

Where TEMPMX, TEMPMN, TEMPM are the maximum, minimum, and mean temperatures (C), respectively. A whole plant grain N sink (NSINK) can then be determined in similar manner to GROGRN.

NSINK = RGNFIL \* GPP \* 1.E-6 (g N/plant)

Since N stress will affect the rate at which plant tissues can mobilize N and supply it to the grain, an N stress factor NDEF4 from subroutine NFACTO is also introduced.

NSINK = NSINK \* NDEF4

If N is present in the plant vegetative tissues (TANC greater than TCNP) the size of the sink is increased. If there is no grain N demand (NSINK = 0) on a day then no grain N accumulation occurs. Two pools of N within the plant are available for translocation, a shoot pool (NPOOL1) and a root pool (NPOOL2). These pools are determined from the N concentration (VANC or RANC) relative to the critical concentration (VMNC or RMNC) and the biomass of the pool (RTWT or TOPWT).

NPOOL1 = TOPWT \* (VANC-VMNC)

and

NPOOL2 = RTWT \* (RANC-RMNC)

Not all of the N contained within these pools can be immediately mobilized. The fraction of these pools which is labile will depend on the N status of the plant. this fraction (XNF) is calculated by considering the N stress index NDEF2 used for vegetative growth and senescence.

XNF = 0.15 + 0.2 \* NDEF2

The labile fraction will range between 15% and 35% of each of the pools depending on the plant N status. The labile poos can be calculated as:

For tops:

TNLAB = XNF \* NPOOL1

and roots:

RNLAB = XNF \* NPOOL2

The total N available for translocation (NPOOL) is the sum of these two labile pools. When NPOOL is not sufficient to supply the grain N demand (NSINK), NSINK is reduced to NPOOL. If NSINK is greater than that which can be supplied by the tops (TNLAB), then TNLAB is removed from TOPSN and the remaining NSINK which must come from the root pool (RNOUT) is calculated. If (NSINK.GT.TNLAB) Then

TOPSN = TOPSN - TNLAB

RNOUT = NSINK - TNALB

TNLAB = 0

ROOTN = ROOTN - RNOUT

When NSINK is less than TNLAB it can be totally satisfied from the shoot pool and the root pool need not be modified.

TOPSN = TOPSN - NSINK

Following the removal of N from shoot and root pools the simulated tissue concentrations (VANC and RANC) are updated. The total amount of N contained in the grain can then be accumulated.

GRAINN = GRAINN + NSINK

The grain nitrogen concentration will vary daily but is only calculated at the end of the simulatin run (in subroutine PHENOL) as:

GNP = GRAINN/GRNWT

These procedures together with the remainder of the growth routine and the N deficiency indices can provide several pathways by which N stress during grain filling can affect grain yield and grain protein content. First, as N is removed from the vegetative tissues NFAC will become lower. This will in turn lower NDEF4 and lower the sink size for N thus providing for the capability of reduced grain N concentration. Lowering NFAC will also lower NDEF1 which will cause the rate of crop photosynthesis to fall thus lowering the assimilate available for grain filling. A declining NFAC will also speed the rate of senescence which will reduce the leaf area available for photosynthesis. Different temperature regimes during grain filling will also affect the final grain N concentration since the function for RGNFIL is more sensitive to temperature than RGFILL. Soil water stress during grain filling can also increase the grain N concentration since SWDF1 will reduce photosynthesis, lowering assimilate availability and thus not diluting grain N as much as would occur in an unstressed crop.

CHAPTER 5 OUTLINE

5.1 Description of Model Inputs

Soil Water Inputs

Genetic Inputs

Nitrogen Inputs

Management Inputs

Weather Inputs

5.2 Measurement of Model Inputs

5.3 Methods for Approximating Model Inputs

Soil Water Parameters

Solar Radiation

Weather Generator

Genetic Coefficients

Soil Nitrogen Inputs

5.4 Structure of Model Input Files

Overview

Structure for Model Directory Files

Structure for Model Input Data Files

5.5 Methods for Generating Model Input Files

The standard input and output files were developed after careful study of the three existing models being adapted for IBSNAT use: CERES-Maize (Jones and Kiniry 1986), CERES-Wheat, and SOYGRO V5.0 (Wilkerson et al. 1985). Each of thses models uses daily weather data, the same soil water balance model (Ritchie 1985), and similarly detailed descriptions of crop phenological development, growth, and yield (Jones and Kiniry 1986; Wilkerson et al. 1985). However, inputs and outputs were initially different and changes were required in each model as it was adapted for use in the DSSAT.

The input and output files for the CERES-Wheat model is organized into four types. a user-friendly interface for the wheat model allows users to select an experiment and then select any or all treatments from the experiment for simulation. Thus, experiments reported in the MDS can easily be simulated for comparison with observed data. Users may also elect to modify treatment conditions to evaluate "what-if" questions. For example, different weather, soil, cultivar, planting date, irrigation management, row spacing, and nitrogen fertilizer management can be changed interactively. Simulated results can then be plotted from any of the runs for comparison with real experimental treatments or for evaluation of hypothetical treatments.

The first type of file has information which identifies experimental data (EXP.DIR) and weather data (WTH.DIR). A second group of files provides input data for crop genetic coefficients, weather, soil, and management information for all of the treatments of an experiment (FILE1,FILE2,...,FILE0). The third type of file contains field-measured data extracted from the MDS for comparison with simulated results for all experimental treatments (FILEA, FILEB). The fourth file type contains output results

# Chapter 5

# Model Inputs

## Determining the Genetic Coefficients

Unless the six genetic coefficients for the varieties to be used have already been determined and are available from the genetics file (see Table 2), they will need to be estimated from experimental data. If no data are available and you wish to run the model, some approximate suggestions will be made. Phasic development in the model must be approximately right before other parts of the model can be expected to work properly, because the duration of crop growth is usually proportional to productivity. The date of anthesis or a similar phenological event, such as ear fully emerged, must come from a test data set in which air temperature was measured. Because the date of anthesis for plants in a field varies considerably, recorded dates of anthesis are subject to error. Thus, having the date of 50% anthesis will help to make accurate determinations of model coefficients. Also, temperature values used in evaluating the phasic development at a site could be incorrect because of a bias in the measuring equipment. For example, the instrument may be some distance from the experimental site, or our assumption regarding the average temperature of the air, being similar to the plant growing point temperature, may be inaccurate under certain circumstances.

Table 2. Genetic Coefficients Ranges and First Try Values.

Parameter Range Notes

P1V 1 = Winter wheat These values usually work for varieties

3 = Spring wheat characterized as winter/spring type except

2 = Intermediate type in regions such as subtropical areas where vernalization of fall sown winter wheat may be marginal. For those areas and a determined intermediate type such as Ralle, a value of 2 can be chosen.

P1D 1 - 5 Use smaller values for varieties with less photoperiod sensitivity; larger values for more sensitive varieties.

P5 1 - 5 Parameters are converted within the model to values which correspond to the length of the grain filling period in oCd, which ranges from 430 - 520 oC. If this is measured, use: P5 = (X oC1 - 430) / 20 to find the correct parameter value.

G1 1 - 5 Use larger values if the variety has above average number of kernels per ear; use smaller values for below average kernel number varieties.

G2 1 - 5 Use larger values for varieties with heavier kernels and smaller values for smaller kernel weight.

G3 1 - 5 Use larger values for varieties with heavier stems; smaller values for smaller varieties.

**How to Determine the Parameters**

1. Run the model with first try values, which are 3 for P1D, P5, G1, G2, G3. Determine whether the variety is a winter or spring type, or choose the values of a variety which is close to the employed variety or one adapted to the same environment.

2. P1V and P1D are to be checked first, because they govern the phasic development of the crop. If the dates of anthesis and maturity, or other major events are simulated correctly, P1V and P1D have the correct values. If predicted dates are early, P1D should be increased for another trial run. Likewise, if the model date is late, the P1D value should be decreased. The values should be only those as given in the table. If the measured dates still contain an error when limiting value is tried, then some other factor, probably the value for PHINT, is contributing to the problem of simulating the anthesis date. The PHINT value can be changed if there is uncertainty about it, but it must also not go out of the range of reality. A user should check the accuracy of the temperature data entries if these procedures do not allow proper estimation of time of anthesis using the proper genetic parameters.

3. To check P5 one must measure the duration of grain fill by sampling individual kernels. Unless the variety under consideration is not known for unusually short or long grain filling duration, the value of 480 degree days should be satisfactory. Often the approximated date of maturity from visual observations is a few days later than the end of grain filling, so that if a date of maturity is recorded from phenological observations, the dates shown in the output for maturity will likely be a few days earlier.

4. The values of G2 and G3 can be changed realistically only if the duration of the entire growth cycle, final biomass and grain yield are approximately correct in the trial run and there was not much stress during the crop growth cycle. If the value of simulated GPSM (grains per square meter) is small, G3 should be increased; if it is large, G3 should be decreased. The new G3 value can be obtained by multiplying the original value used for G3 in the simulation by the ratio of the measured GPSM to the simulated GPSM.

5. For modern varieties of wheat, G2 and G3 are inversely related. G3 is proportional to final kernel weight, thus larger values should produce larger grains in simulations. However, because of the possible problems of assimilate supply to fill grains toward the end of grain filling period, it is often not possible to obtain larger grain size by increasing G3. As with other genetic coefficients, the values of G2 and G3 should not be taken out of range to try to obtain a fit with experimental data. Some other problem could be causing the error.

6. The value of G4 is related to size of individual stems. Thus larger values are related to larger stem varieties. The best strategy for obtaining a good value for G4 is to check the number of ears obtained in the first simulation with the number of ears measured. If the simulated value is too large, the stem weight parameter G4 is too small; if the simulated number of ears is too small, G4 should be decreased.

Accuracy for the G2, G3 and G4 parameters is necessary if yield components are to be successfully simulated. However, if getting ear number, grain number, and grain weight are not too critical, the yield usually will not be strongly influenced by the choice of the parameters, at least for the more modern varieties, unless the value chosen for G2 is too small.

When any of the genetic parameters are fit from experimental data, the accuracy of the model cannot be validated with the same data set. However, if only the duration constants (P1, P2, P3) are fit, the biomass and yield parts of the model can be properly tested. The most desirable strategy is first to grow a crop to obtain the proper genetic coefficients, and then test the model with another year's crop or another sowing date or location.

**5.4 STRUCTURE FOR MODEL INPUT FILES**

**EXP.DIR: Experiment File Directory**

**Description**

The experiment file directory was developed to allow great flexibility in retrieving data needed to simulate various experiments from different locations and different years. This file contains the names of all input and output data files associated with a particular experiment for a crop. For each experiment in the file, three lines of information are required, and there must be a blank space before each field, except before the first field on each line, to ensure readability of this file. On the first line, the experiment identifier (8 characters) specifies the institute code, site code, year of experiment, and experiment number. After skipping one space, the next 40 characters briefly describe the experiment. The next two 12-character fields on line one identify the weather file name associated with this experiment (FILE1) and the name of the soil profile file (FILE2). On the second line of the experiment directory file, there are six 12-character fields which identify the names of files FILE4 through FILE9 for this experiment. On the third line, two 12-character fields identify the names of the validation files FILEA and FILEB, and four 7-character fields identify output files OUT1 through OUT4. If more than one experiment is to be simulated, three lines, equivalent in content to the first three described above, are appended to the EXP.DIR file for each experiment.

An example of EXP.DIR follows for a 1981 experiment in Ashland, Kansas. An EXP.DIR is needed for each experiment and the wheat identifier is appended to the front of this file to signify this is for wheat.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1

EXPID A8 Experiment identifier.

EXPDE 1X,A40 Experiment description.

FILE1 1X,A12 Daily weather data file name.

FILE2 1X,A12 Soil profile file name.

Format for line 2

FILE4 A12 Soil nitrogen dynamics properties file name.

FILE5 1X,A12 Soil profile initial conditions file name.

FILE6 1X,A12 Irrigation management data file name.

FILE7 1X,A12 Nitrogen fertilizer management data file name.

FILE8 1X,A12 Crop management data file name.

FILE9 1X,A12 Genetic coefficients file name.

Format for line 3

FILEA A12 Measured summary data file name.

FILEB 1X,A12 Measured seasonal data file name.

OUT1 1X,A12 File name for output file 1.

OUT2 1X,A12 File name for output file 2.

OUT3 1X,A12 File name for output file 3.

OUT4 1X,A12 File name for output file 4.

**WTH.DIR: Weather File Directory**

**Description**

This file has a list of all weather data file names along with information on location, and beginning and ending month of weather data in the file. Weather file names include institute and site code identifiers, beginning month of weather, number of months of weather records, and the year in which the data starts. For example, KSAS0517.W81 is the name of the weather data file for Kansas State University (KS), at the Ashland site (AS), beginning with May data (05), and containing 17 months of data (17) beginning in 1981 (81). Weather data in a file can start in one year and go into a second year. KSAS0517.W81 has data starting in May, 1981 and continuing for 17 months through 1982. This WTH.DIR file should contain the file names of all weather data that a user would need to simulate actual or hypothetical experiments. An example of this file is given below with reference to two weather data sets.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

WTHID A4 Weather station ID.

WTHDES 1X,A40 Weather station description.

BEGDATE A8 Beginning date in weather file.

ENDDATE 1X,A8 Ending date in weather file.

FILE1 1X,A12 Weather file name.

**Example of the Weather Directory File, WTH.DIR**

**STRUCTURES FOR MODEL INPUT DATA FILES**

**FILE1: Daily Weather Data**

**Description**

Daily weather data must be available in FILE1 for all days of the growing season (minimum requirement), beginning with day of planting and ending at crop maturity. Ideally, the file should contain weather data collected both before planting and after crop maturity. Then, the simulation could start before planting so that soil processes would be simulated. Initial conditions for the soil should coincide with the first day of simulation. Additional weather data also allows users to select alternate planting dates or longer duration crop varieties for model sensitivity analysis. On the first line of this file, the institute and weather station site code identifiers are listed, followed by latitude. Provision is made for compatibility with other models utilized by the IBSNAT Project. Some require as extra inputs the following:

-longitude

-a conversion coefficient (PARFAC) to convert total radiation to photosynthetically active radiation (PAR)

-an indicator as to whether PAR is available in the data file (PARDAT).

For further details, refer to IBSNAT Technical Report 5.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1 of weather data file

INSTW A2 Code for institute ID.

STATW A2 Code for weather station ID.

XLAT 1X,F6.2 Latitude of station.

Format for all other lines of weather data

INSTW A2 Code for institute ID.

STATW A2 Code for weather station ID.

IYR 1X,I2 Year for which weather data is being read.

JUL 1X,I3 Julian date of weather record in data file.

SOLRAD 1X,F5.2 Daily total solar radiation, MJ/m2.

XTMAX 1X,F5.1 Daily value of maximum temperature, oC.

XTMIN 1X,F5.1 Daily value of minimum temperature, oC.

XRAIN 1X,F5.1 Daily total precipitation, m/day.

**Example**

This example has weather data from an Ashland experiment:

**FILE2: Soil Profile Properties**

**Description**

Soil profile properties are used in the soil water, nitrogen, and root growth sections of the crop models. The first line of data in this file contains space for a soil number, a pedon number, and a soil classification name. With the exception of the soil number, this can be left blank and not affect the functioning of the model. The second line of data contains soil properties that do not vary with depth, such as surface albedo, runoff curve number, etc. Starting with line 3, one line of data is used for each layer in the profile. After the lines with properties for all layers, a line with a "-1" in the first field is required to indicate the end of data for a soil. The number of layers in this file and the thickness of each layer must be consistent with the initial conditions in FILE5. Default initial conditions for the soil are in FILE2 and will be used if FILE5 is not available. Properties for several soils are input into this file by appending data from each available soil, each with its own sequence number and pedon number. This file may contain properties for several soils with the same soil classification. Model users can use this format and manually input their own values for a soil. LL(L), DUL(L), SAT(L), can be determined from other soil properties if they have not been determined directly. Procedures for doing this are described in 5.XXXX\_\_\_\_\_\_\_\_\_\_.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1

IDUMSL 1X,I2 Number assigned to a soil type.

PEDON 1X,A12 Pedon number.

TAXON 1X,A60 Soil classification name.

Format for line 2

SALB F6.2 Bare soil albedo, no units.

U 1X,F5.2 Upper limit of stage 1 soil evaporation, mm.

SWCON 1X,F6.2 Soil water drainage constant, fraction drained per day.

CN2 1X,F6.2 SCS curve number used to calculate daily runoff.

TAV 1X,F5.1 Annual average ambient temperature, oC.

AMP 1X,F5.1 Annual amplitude in mean monthly temperature, oC.

DMOD 1X,F3.1 Zero-to-unity factor whichreduces the rate constant for mineralization of the humus pool for soils which are poor mineralizers due to chemical or physical protection of the organic matter (default = 1).

Format for line 3 through n

DLAYR (L) F6.0 Thickness of soil layer L, cm.

LL (L) 1X,F6.3 Lower limit of plant-extractable soil water for soil layer L, cm3/cm3.

DUL (L) 1X,F6.3 Drained upper limit soil water content for soil layer L, cm3/cm3.

SAT (L) 1X,F6.3 Saturated water content for soil layer L, cm3/cm3.

SW (L) 1X,F6.3 Default soil water contentfor soil layer L, cm3/cm3.

WR (L) 1X,F6.3 Weighting factor for soil depth L to determine new root growth distribution, no units.

BD (L) 1X,F5.2 Moist bulk density of soil in soil layer L, g/cm3.

OC (L) 1X,F5.2 Organic carbon concentration in soil layer L, %.

NH4 (L) 1X,F4.1 Default soil ammonium in soil layer L, mg elemental N/kg soil.

NO3 (L) 1X,F4.1 Default soil nitrate in soil layer L, mg elemental N/kg soil.

PH (L) 1X,F4.1 Default pH of soil in soil layer L in a 1:1 soil: water slurry.

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

These are not required by the model for calculation purposes but function in the labelling of outputs and sections of the files.

**Example**

**FILE3: Reserved For User Application**

**FILE4: Soil Nitrogen Balance Parameters**

**Description**

These are treatment-specific parameters required by the wheat model that use the nitrogen dynamics component. For this file, the parameters may also depend on the treatments of the experiment. Therefore, one set of these data is needed for each treatment of an experiment and they must be recorded consecutively. This file is not needed if the model is to be run with the assumption that nitrogen is nonlimiting.

Data Formats

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

INSTS A2 Code for institute ID.

SITES A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

TRTNO 1X,I2 Treatment number.

STRAW 1X,F5.0 Weight of organic residue of previous crop and/or added green manure, kg/ha.

SDEP 1X,F5.0 Depth of surface residue incorporation, cm.

SCN 1X,F5.0 C:N ratio of surface residue of previous crop, kg C/kg N (default = 75.0).

ROOT 1X,F5.0 Dry weight of root residue of previous crop, kg/ha (default = 500).

**Example**

FILE5: Soil Profile Initial Conditions

Description

FILE5 contains initial conditions for soil profile water and nitrogen dynamics submodels. These initial conditions specify the values of water content, ammonium, nitrate, and pH in each layer at the start of the first day of the simulation. Thus, the simulation must be started on the day for which the initial conditions are specified, even if the planting date is later. Soil profile initial conditions must be specified for a date before planting, or at the latest, on the date of planting which is input in FILE8. The thickness of each layer and the number of layers in this file must correspond exactly with those in FILE2. The first line of data in FILE5 consists of treatment number and an experiment code identifier. Then, there will be one line of data for each soil layer and a "-1" on the line immediately following the data for the last soil layer. This file will have data for each treatment of an experiment at a site, with the treatment being identified on the top line of each consecutive set.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1

TRTNO I2 Treatment number.

INSTS 1X,A2 Code for institute ID.

SITES A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

Format for all other lines

DLAYR (L) F6.0 Depth of layer L, cm.

SW (L) 1X,F6.3 Soil water content of soil layer L, cm3/cm3.

NH4 (L) 1X,F4.1 Soil ammonium in soil layer L, mg elemental N/kg soil.

NO3 (L) 1X,F4.1 Soil nitrate in soil layer L, mg elemental N/kg soil.

PH (L) 1X,F4.1 pH of soil in soil layer L in a 1:1 soil: water slurry.

**Example**

**FILE6: Irrigation Management Data**

**Description**

For each treatment in an experiment at a site, the amounts and dates of irrigation events are contained in FILE6. The first line of data for each treatment in the file must contain the treatment number and the experiment code identifier. Then, one line of data is required for each irrigation event. After all irrigation events have been entered for a treatment, a "-1" is entered in each field to signal the end of data for the treatment. Data for the second treatment and subsequent treatments are stacked below that of the first treatment, and data for all treatments are thus contained in this file.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1

TRTNO I2 Treatment number.

INSTE 1X,A2 Code for institute ID.

SITEE A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

Format for all other lines

IDAY (J) I4 Day of year of irrigation event J.

AIRR (J) 1X,F4.0 Amount of irrigation added on IDAY (J), mm.

Example

FILE7: Fertilizer Management Data

**Description**

This file is organized similarly to FILE6. For each fertilizer application, one line of data with the four variables listed below must be supplied to FILE7. Since fertilizer applications may vary among treatments, data for each treatment will be sequentially listed in this file. Each set will have the treatment number and experiment code identifier on its top line of data. Following the last entry for each treatment, a "-1" in each field will be used to signal the end of that treatment's data. This file is not required if the model is being run with the assumption that nitrogen is nonlimiting.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1 of each treatment

TRTNO A2 Treatment number.

INSTE 1X,A2 Code for institute ID.

SITEE A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

Formats for all fertilizer application events

FDAY (J) I4 Day of year of nitrogen fertilizer application J.

AFERT (J) 1X,F5.1 Amount of fertilizer nitrogen added on FDAY (J), kg N/ha.

DFERT (J) 1X,F5.1 Depth of incorporation of fertilizer application on FDAY (J), cm.

IFTYPE (J) 1X,I2 Code number for type of fertilizer as specified in Appendix (xxxx)......

**Example**

**FILE8: Treatment Management Data**

Description

FILE8 contains crop management data for each treatment averaged over all replications. Two lines of data are required for each treatment of an experiment and must be in consecutive order. On the first line, the experiment code identifier, a brief description of the treatment, the soil number for the treatment, and the cultivar used in the treatment are designated. On the second line, day to begin simulation, planting date, row spacing, and other management data for the treatment are specified. The first pair of lines in this file are for treatment 1 of the experiment, the second pair are for treatment 2, and so on.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

Format for line 1

INSTE A2 Code for institute ID.

SITEE A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

TRTNO 1X,I2 Treatment number.

TITLET 1X,A40 Title of treatment.

ISOILT 1X,I4 Soil number for this treatment as described in FILE2.

IVARTY 1X,I4 Cultivar number for this treatment as described in FILE2.

Format for line 2 of each treatment in this file

ISIM I4 Date simulation begins.

ISOW 1X,I3 Sowing date, day of the year.

PLANTS 1X,F6.2 Plant population, plants/m2.

ROWSPC \* 1X,F6.3 Row spacing, m.

SDEPTH 1X,F5.2 Sowing depth, cm.

IIRR 1X,I2 Switch describing irrigation (default = 1).

1: no irrigation applied

2: irrigation applied using field schedule

3: automatically irrigated at threshold soil water

4: assume no water stress, water balance not used

ISWNIT 1X,I2 Switch to indicate if nitrogen routines are used (default = 0).

0: nitrogen subroutines are not used, assumes adequate nitrogen

1: nitrogen subroutines are used

EFFIRR 1X,F6.2 Irrigation system efficiency, fraction.

DSOIL 1X,F5.2 Irrigation management depth, m.

THETAC 1X,F6.1 Available water triggering irrigation, %.

PHINT 1X,F6.2 Phyllochron interval (day degree). Default = 95 (CERES models).

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

\* This is not required by the model but is included for compatibility with IBSNAT models.

**Example**

**FILE9: Genetic Coefficient Data**

**Description**

This file has the name GENETICS.WH9 and contains the genetic coefficients which describe specific characteristics of a cultivar. The file has one line for each cultivar and the complete file is listed in Appendix NN. The file consists of a code number for each cultivar, the cultivar name and the list of genetic coefficients. The appropriate cultivar is selected in a model run by entering the cultivar code number in FILE8. Alternatively a different cultivar can be selected by invoking the menu options. Provision has also been made within the menus to add a new cultivar to a genetics file.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

IVAR I4 Cultivar code number.

VARTY A16 Name of cultivar.

P1V F3.1 Relative vernalization sensitivity (1,2 or 3).

P1D 5X,F4.1 Relative photoperiod sensitivity (0 to 5 scale).

P5 5X,F7.1 Relative duration of grain filling Phase (0 to 5 scale).

G1 F4.1 Relative value of conversion factor for grain number per

unit stem weight (0 to 5 scale).

G2 3X,F4.1 Relative value of maximum possible daily growth rate of a kernel (0 to 5 scale).

G3 3X,F4.1 Relative value for potential dry weight of a single stem and ear at anthesis (0 to 5 scale).

**STRUCTURES FOR MODEL VALIDATION FILES**

**FILEA: Measured Crop Summary Data**

**(May vary by crop)**

**Description**

For each treatment of each experiment, crop experimental data may differ. FILEA contains crop measured field data for each treatment averaged over all replications. The measured field data are needed for the standard outputs which list simulated and measured data side-by-side.

**Data Formats**

Variable Name FORTRAN Format Description

\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_

**Wheat**

INSTE A2 Code for institute ID.

SITEE A2 Code for site ID.

YEAR A2 Year number, last two digits.

EXPTNO I2 Experiment number.

TRTNO 1X,I2 Treatment number.

XYIELD 1X,F7.0 Actual field-measured grain yield dry weight basis, kg/ha.

XGRWT 1X,F7.4 Field-measured kernel dry weight, g/kernel.

XGPSM 1X,F6.0 Field-measured grain number, grains/m2.

XGPE 1X,F4.0 Field-measured grain number, grains/ear.

XLAI 1X,F5.2 Field-measured leaf area index at anthesis, m2/m2.

XBIOM 1X,F6.0 Field-measured aboveground dry biomass at maturity, kg/ha.

XSTRAW 1X,F6.0 Measured straw and chaff dry weight at maturity kg/ha.

IANTD 1X,I3 Field-measured anthesis date, day of year.

MATD 1X,I3 Field-measured physiological maturity date, day of year.

Start line 2

GRPCTN F6.2 Measured nitrogen concentration in grain at maturity, %.

XTOTNP 1X,F5.1 Measured crop nitrogen content at maturity, kg/ha.

XAPTNP 1X,F5.1 Measured stover nitrogen content at maturity, kg/ha.

XGNUP 1X,F5.1 Measured grain nitrogen content at maturity, kg/ha.

**FILEB: Observed Data for Graphics**

**Description**

FILEB is reserved for storage outputs of various parameters for use in graphical displays.

# CHAPTER 6

# MODEL OUTPUTS

The model creates a file, SIM.DIR, which contains the file names of four output files and the titles of the treatments simulated as well as a file name for seasonal observation data. These file names can later be picked up by the graphics program for graphical display of outputs (see User's Guide for details). If a file name was listed for a fifth output file in the experiment directory file (WHEXP.DIR) for risk analysis or multiple-year applications, then the name of this file will also appear in SIM.DIR. If no file name for this (generally OUT5.WH) was entered in WHEXP.DIR then SIM.DIR will not contain this file name.

The five output files for any experiment contain different classes of data. The nature of the outputs in each of these files is described below:

File Number Name Description

1 OUT1.WH Summary output file describing management inputs, crop development, simulated yield, yield components and comparisons with observations.

2 OUT2.WH Simulated crop variables vs. time.

3 OUT3.WH Summary weather data and simulated water balance variables vs. time.

4 OUT4.WH Simulated soil and plant N variables vs. time.

5\* OUT5.WH Summary data for use in risk analysis.

\*Optional output file

In File 1, a one line summary output is written at the end of each growth stage. In Files 2, 3, and 4 output is written to file after every seven days of simulation. Provision has been made within the model to allow the user to interactively select a different output frequency for each of Files 2, 3 and 4 if desired. This is described in more detail in the User's Guide.

## OUTPUT FILE HEADER INFORMATION

Each of the output files commences with a header containing the title used for the simulation run, the identification codes for the institute, and site where the experiment being simulated was conducted. Titles for the experiment, the treatment within the experiment, treatment number and the year the experiment was planted are also printed. The header also identifies the weather data set used, the soil type and the variety used in the experiment. Identical headers are printed in each of the four files for each treatment simulated.

## SUMMARY OUTPUT FILE

When running the model the summary output appears on the screen as the crop is being simulated. Output File 1 is a record of what appears on the screen. After listing the file header information, the latitude, sowing depth and plant population and the genetic constants for the variety simulated are listed. This information is followed by irrigation information if the crop was irrigated. This lists the dates and amounts of each irrigation applied. This information is followed by soil characteristics including: a name for the soil pedon (PEDON), the soil albedo, the upper limit of Stage 1 soil evaporation (U), soil water conductivity (SWCON), and runoff curve number. For each layer in the profile the following information is then displayed: the lower and upper depth boundaries of the soil layer, the lower limit of plant extractable water (LO LIM), the drained upper limit (UP LIM), the soil water content at saturation (SAT SW), the plant extractable soil water (EXT SW), initial soil water content (IN SW), the rooting preference factor (WR), the extractable nitrate (NO3) and ammonium (NH4) in units of mg N/kg soil. All water contents are expressed as volume fractions. Below the layer information, totals for the whole profile where appropriate are displayed. For the water contents these totals are expressed as cm of water and for the nitrogen concentrations the totals are expressed in units of kg N/ha.

If the nitrogen balance is being simulated, the model next lists fertilizer information. For each application, the day of the year, the amount (kg elemental N/ha), the depth of incorporation, and the fertilizer source are listed.

All of the display described so far refers to an "echo" of the inputs required for the simulation run. When running the model this echo can be switched off so that only the summary information generated by the simulation as described below is displayed on the screen. Regardless of whether the echo is displayed on the screen or not it is written to the output file. After the echo, the program prints a message indicating the day simulation began.

Once simulation has commenced, one line of summary information is displayed at the end of each growth stage. These data include the day of the year, the accumulated thermal time since planting (CDTT), the description of the ontogenetic stage, the above-ground biomass (BIOM,g/m2), leaf area index (LAI), nitrogen uptake in the above-ground vegetative biomass (NUPTK,kg N/ha), the concentration of N in the above-ground vegetative biomass (N%,%), the cumulative evapotranspiration (CET,mm), the cumulative precipitation (RAIN,mm) and plant extractable soil water in the soil profile (PESW). RAIN and CET are accumulated from the beginning of the simulation until germination. After germination RAIN and CET are both initialized to zero, their values then represent the cumulative ET and precipitation occurring after germination. When the simulation reaches the terminal spikelet stage of growth (T SPKLT) the number of days the crop underwent vernalization (VE DAYS) is printed. At the end of ear growth, the number of ears (EARS) per square meter is also printed. At maturity the grain yield in kg/ha and bushels/acre, the grains per square meter (GPSM) and the dry weight of a single kernel (mg) are printed.

Next the model prints a comparison table of predicted and observed values of: the date of anthesis,the maturity date, the grain yield (kg/ha), the kernel weight (mg), the number of grains per square meter, the number of grains per ear, the maximum leaf area index, final above-ground biomass (kg/ha), the weight of straw (kg/ha), the nitrogen concentration in the grain (%), the total above-ground nitrogen uptake (kg N/ha), the straw N uptake (kg N/ha), and the grain N uptake (kg N/ha). When running the model an option exists to bypass displaying this table. If the menus were accessed during the model run, a message is printed indicating the comparison of predicted and observed yield may not be valid.

The model next prints a summary of the water and nitrogen stresses which occurred during each of the growth stages of the crop. CSD1 and CNSD1 refer to the cumulative stress indices for water and nitrogen respectively for photosynthesis. CSD2 and CNSD2 refer to the water and nitrogen (respectively) cumulative stress indices for extension growth processes. When these indices have a value of unity it implies the maximum amount of stress occurred during that growth stage and a zero value implies that no stress occurred during that period (Fig. 6.1)

Fig. 6.1

## CROP GROWTH OUTPUT FILE

This file can be displayed when a model run has been completed. The model prints the header information at the beginning of the file and the growth information is written in subroutine OUTGR. The interval at which output is written to this file has a default value of seven days but this may be changed by accessing the output frequency menu when running the model. The following information is written to the file: day of the year, the cumulative thermal time elapsed since the beginning of the growth stage (SDTT, day degrees), above-ground biomass (BIO, g/m2), tillers per meter square (TPSM), leaf area index (LAI), root weight (ROOT, g/plant), stem weight (STEM, g/plant), grain weight (GRAIN ,g/plant), leaf weight (LEAF, g/plant), root depth (RTD, cm), plant top fraction (PTF), and root length density (RLV, cm root/cm3 soil) in layers 1, 3 and 5 in the profile. Fig. 6.2 is an example of the printed output from OUT2.WH.

## SOIL WATER OUTPUT FILE

This file (Fig. 6.3) can be displayed when a model run has been completed. The model prints the header information at the beginning of the file. This file is written in subroutine OUTWA. The interval at which output is written to this file has a default value of seven days but this may be changed by accessing the output frequency menu when running the model. The following information is written to the file: day of the year, plant transpiration (EP,mm), evapotranspiration (ET,mm), potential ET (EO,mm), solar radiation (SR,MJ/m2), maximum temperature (MAX, oC), minimum temperature (MIN,oC), total precipitation over the interval (PREC,mm), the volumetric soil water content in each of the top five layers (SW1-SW5) and the total plant extractable soil water in the soil profile (PESW,cm).

**Fig. 6.2**

**Fig. 6.3**

## SOIL AND PLANT NITROGEN OUTPUT FILE

This file (Fig. 6.4) can be displayed when a model run has been completed. The model prints the header information described previously at the beginning of the file. This file is written in subroutine OUTNU. The interval at which output is written to this file has a default value of seven days but this may be changed by accessing the output frequency menu when running the model. The following information is written to the file: day of the year, plant tops N concentration (%), N deficiency index (NFAC), total N uptake by above ground plant parts (TOT N UPTK, kg N/ha), N uptake into grain (GRAIN UPTK, kg N/ha), soil concentrations of nitrate in the upper five soil layers (ug N/g soil), and soil concentrations of ammonium in the upper three soil layers (ug N/g soil).

Fig. 6.4

OUTPUT FILE 5 (OUT5.WH)

This file will only be created when a name is listed in the experiment directory file. The file contains one line of summary information for each year of simulation. This file is compatible with the strategy evaluation program of IBSNATs Decision Support System for Agrotechnology Transfer. The file contains the following entries:

ENTRY INTERPRETATION

Crop Code This will always be WH:

A-M Days Number of days from anthesis to physiological maturity

E-M Days Number of days from emergence to physiological maturity

NLOSS Nitrogen lost from the profile (kg N/ha) by denitrification and leaching (nitrate moving through a layer at 1 meter depth is deemed lost for this purpose)

NIT STRS 3 Nitrogen stress index for growth stage 3

NIT STRS 5 Nitrogen stress index for growth stage 5

NUPTK Aboveground crop nitrogen uptake (kg N/ha)

NIRR Number of irrigations made to the crop

WAT STRS 1 Water stress index for growth stage 1

WAT STRS 5 Water stress index for growth stage 5

CET Cumulative evapotranspiration (mm) since emergence

RAIN Cumulative rainfall (mm) since emergence

BIOMASS Aboveground crop biomass (Tonnes/ha)

YIELD Grain Yield (Tonnes/ha)

PLANTS Plant population (plants/sq meter)

NFT Number of fertilizer applications made

NRATE Total amount of fertilizer N added (kg N/ha)

TITLE Treatment title

CHAPTER 7

**A STEP-BY-STEP PROCEDURE TO RUN THE CERES-WHEAT**

**MODEL ON A PERSONAL COMPUTER**

List of files on the distribution diskettes.

REQUIREMENTS

To run the CERES-Wheat model, you must have the following:

IBM PC or compatible with at least 256K RAM Memory DOS (Disk Operating System) 2.0 or higher.

SYSTEM PREPARATION

A change must be made to a DOS file, CONFIG.SYS, in order to run the model. The CONFIG.SYS file must have a FILES=20 statement to run the model. By running the procedure described below, a CONFIG.SYS file will be created if one does not exist. If a CONFIG.SYS file does exist, it will be altered by adding the FILES=20 statement. If a CONFIG.SYS file does exist and has the FILES=20 statement, then proceed to "Running the Model". If your DOS files are on diskette and you have a single disk drive, refer to the following section "Preparing A Single Drive System". If your DOS files are on diskette and you have two disk drives, refer to the following section "Preparing A System With Two Drives." If your DOS files are on a hard disk, refer to the section "Preparing A Hard Disk System".

**Preparing a Single Drive System**

Using your DOS diskette, make a backup copy of your DOS diskette. With the DOS diskette in A:, type "DISKCOPY A: A:" at the A> prompt. When instructed, place a blank diskette in drive A:. After completing the copy, place the original DOS diskette in a safe place and use the backup copy. Be sure the backup DOS diskette is not write-protected. Place the diskette labeled " " in drive A: and type "CHANGE" at the A> prompt. When instructed, place the backup copy of DOS in drive A:. When you receive the A> prompt, reboot your system by placing the backup copy of DOS in drive A: and pressing the keys <CTRL>, <ALT>, and <DEL> at the same time. Use the backup copy of DOS to boot your system each time. Continue now to the section "Running the Model".

P**reparing a System With Two Disk Drives**

Using your DOS diskette, make a backup copy of your DOS diskette. With the DOS diskette in A: and a blank diskette in drive B:, type "DISKCOPY A: B:" at the A> prompt. After completing the copy, place the original DOS diskette in a safe place and use the backup copy. Be sure the DOS diskette is not write-protected. Place the diskette labeled " " in drive A: and the DOS diskette in drive B:. At the A> prompt, type "CHANGE". When you receive the A> prompt, reboot your system by placing the backup copy of DOS in drive A: and pressing the keys <CTRL>, <ALT>, and <DEL> at the same time. Use the backup copy of DOS to boot your system each time. Continue now to the section "Running the Model".

**Preparing a Hard Disk System**

With your hard disk at the subdirectory where the COMMAND.COM file is, place the diskette labeled " " in drive A:. At the A> prompt, type "CHANGE". When you receive the A> prompt, reboot your system by pressing the keys <CTRL>, <ALT>, and <DEL> at the same time. Continue now to the section "Running the Model".

**Running the Model**

Before running the model, make a backup copy of the diskette labeled "CERES-Wheat Model". The system should be rebooted if you have not already done so. Place the backup diskette in drive A:, making sure it is not write-protected. At the A> prompt, type "WHEAT". The following screen will appear:

After pressing return, a list of experiments to be simulated comes up on the screen:

Choose a selection. If you do not choose a selection (hit return), the default (Experiment 1) will be chosen. After a selection has been made, a list of available treatments for that experiment appears:

If you do not choose a treatment, the default (Treatment 1) will be chosen. After choosing a treatment, a list of run-time options comes up:

Choosing option 0 will run the simulation using all the input data in its existing form. Option 1 enables alteration to the frequency of the output for crop growth (Output File 2), water balance (Output File 3), and nitrogen balance (Output File 4). The default setting is, as shown below, seven days:

Using Option 1, the output frequency for these three output files can be altered. Option 2 will produce the following screen:

Option 2 enables modification of almost all of the input parameters interactively. A word processor is not needed to pose "what if" questions. When any option between 1 and 9 is chosen, further menus appear to help modification of the input data. Each of these menus features a terminator enabling return to the main selection menu.

Option 1 of the interactive modification menu allows the planting date to be changed:

Option 2 of the menu allows the plant population to be changed:

Simulation of nitrogen balance can be switched off or on using Option 3:

Simulation of nitrogen balance can also be switched back on using

Option 3:

Irrigation data can be added or modified using Option 4. The method of irrigation can also be changed:

The user would then choose Option 2 of Option 4 to add data to create a field schedule. Fertilizer data can be modified or added using Option 5:

The changes can then be viewed:

Option 6 allows a choice of a new variety. All current varieties available are printed out and then a choice can be made of a new variety. For the purposes of this example, only the first and last screens of Option 6 are shown:

A new variety can be created and used for the simulation only or can be written back out to the existing genetics coefficient file:

Option 7 enables selection of a different soil, as seen below :

The following parameters can be modified or simply looked at using Option 2 of Option 7:

Layer data can also be modified or viewed using Option 2 of Option 7:

Note that a "0" was entered at how many layers you want to modify, so as to check or "view" the parameter OC. Different weather data can be chosen using Option 8. Please note that the weather data chosen should have the same dates as the experiment :

Soil profile parameters can be checked and/or modified using Option 9:

The soil profile parameters can be viewed or modified as previously shown with Option 7. Soil moisture can be initialized to a percentage of whole profile storage by choosing Option 2 of Option 9:

Crop residue parameters can be modified using Option 3 of Option 9:

Option 10 of the interactive menu displays key input data on the screen for checking prior to running the simulation. Option 11 terminates data modification and runs the simulation. Option 12 terminates data modification, abandoning all previous changes, and returns back to the choosing an experiment menu. During the simulation run, certain error messages may appear if a file is not in the correct format or if data is missing. Below are some examples of possible error messages:

# CHAPTER 8

# VALIDATION OF THE MODEL

## VALIDATION PROCEDURES

Testing model performance during development of a model usually results in calibration, which is, according to Penning de Vries (de Vries and von Laar, 1982) a "very restricted form of evaluation," and "adjustment of some parameters such that model behavior matches one set of real world data." It can "degrade simulation into curve fitting."

Before any model can be used with confidence, adequate validation or assessment of the magnitude of the errors that may result from their use should be performed. Model validation, in its simplest form, is a comparison between simulated and observed values.

Beyond comparisons, there are several statistical measures available to evaluate the association between predicted and observed values, among them the correlation coefficient (r) and its square, the coefficient of determination (r2). Willmott (1982) has pointed out that the main problem with this analysis is that the magnitudes of r and r2 are not consistently related to the accuracy of prediction where accuracy is defined as the degree to which model predictions approach the magnitudes of their observed counterparts.

Test criteria have been separated into two groups, called summary measures and difference measures. Summary measures include the mean of observed values (0) and predicted values (P), the standard deviations of observations (So) and the predictions (Sp), the slope (a) and intercept (b) of the least-squares regression:

Pi = a + b \* 0i

In addition, an index of agreement (d) (Willmott, 1982) was calculated as follows:

n n

2 2

d = 1 - [ S (P - O ) / S (|P'| + |O'|) ], 0 < d < 1

i i i i

i=1 i=1

\_ \_

where P' = P - O and O' = O - O

i i i i

Though (d) is meant to be used mainly to determine the relative superiority of alternative models, it can be valued as a descriptive parameter of model performance. The more (d) approaches 1, the more accurate the model.

While summary measures describe the quality of simulation, difference measures try to locate and quantify errors. The latter includes the mean absolute error (MAE), the mean bias error (MBE), and the root mean square error (RMSE). They all are calculated according to Willmott (1982) and based on the term (Pi - 0i):

A) Mean Absolute Error (MAE):

n

MAE = S | Pi - 0i | / n

i=1

B) Mean Bias Error (MBE):

n

MBE = S (Pi - 0i) / n

i=1

C) Root Mean Square Error (RMSE):

n

RMSE = S (Pi - 0i)2 / n

i=1

MAE and RMSE indicate the magnitude of the average error, but provide no information on the relative size of the average difference between (P) and (0). MBE describes the direction of the error bias. Its value, however, is related to magnitude of values under investigation. A negative MBE occurs when predictions are smaller in value than observations.

In the test of data sets without N routines, attention was focused on the unsystematic error (RMSEu) as in the system:

MSE = MSEs + MSEu

For a good model, the unsystematic error RME should approach RMSE, with RMSEs approaching 0/, which is what could be observed.

In addition to these basic tests, a number of procedures were tested using the data sets with N routines only. These are:

o A simple regression technique, suggested by Dent and Black (1979) combined with an F-test to evaluate the null hypothesis of the slope and intercept simultaneously, being different from zero and unity, respectively.

o A statistic to determine model accuracy as defined by Freese (1960).

o A 5 percent critical error as defined by Reynolds (1984).

For results of the above mentioned tests, see Tables 1 and 2.

The parameters examined in the statistical evaluation were:

1. Anthesis date

2. Maturity date

3. Leaf area index (LAI) at maximum

4. Total above ground dry matter at maturity

5. Grain yield

6. Individual grain weight at maturity

7. Number of grains per m2 at maturity

8. Dry matter at anthesis

9. N uptake by the crop at anthesis

10. N uptake in the above ground plant parts at maturity

11. N content of the grain

12. Grain protein percentages

Parameters 1 through 7 were evaluated without using N routines (see Tables 3 and 4), whereas parameters 4 through 12 specially referred to aspects of the N routines to be tested (see Tables 1 and 2).

Table 1. Summary Measures for Data Sets with N Routines

\_ \_

Variable Units N O P So Sp a b R d

Dry matter kg/ha 222 10,313 11,719 3,375 3,897 189.3 1.118 0.82 0.86

Grain yield kg/ha 240 3,953 4,227 1,716 1,719 145.6 1.033 0.84 0.91

Total N uptake kg N/ha 223 110 121 47 45 7.0 1.042 0.72 0.83

Grain N uptake kg N/ha 215 84 87 34 31 4.4 0.996 0.74 0.85

Grain protein percent 215 12.3 11.7 2.95 3.55 0.198 0.939 0.55 0.74

GPSM no. 152 12,381 11,861 4,668 5,324 362 0.929 0.63 0.78

Kernel weight mg 134 33.6 37.9 7.02 8.40 0.998 1.096 0.34 0.59

App recovery percent 137 45.7 43.4 29.4 25.68 8.37 0.767 0.37 0.65

Table 2. Difference Measures for Data Sets with N Routines

Variable Units N MAE MBE RMSE RT E\*

Dry Matter kg/ha 222 2,248.1 1,405.6 2,648.2 13.06 480.9

Grain yield kg/ha 240 806.1 274.4 1,024.2 15.39 186.5

Total N uptake kg N/ha 223 28.6 11.5 36.3 22.43 65.9

Grain N uptake kg N/ha 215 19.4 3.5 24.0 18.64 43.6

Grain protein percent 215 2.4 -0.6 3.2 18.65 5.8

GPSM no. 152 3,462.3 -520.8 4,355.4 22.43 778.6

Kernel weight mg 140 8.1 4.2 9.9 12.00 17.6

App recovery percent 137 23.5 -2.3 31.2 69.48 55.5

Note: N = Number of observations.

O = Mean of observations.

P = Mean of predictions.

SO = Standard deviation of observations.

SP = Standard deviation of predictions.

a = Intercept term from regression of predicted on observed.

b = Slope term from regression of predicted on observed.

R = Regression coefficient.

D = Index of agreement (Willmott, 1982).

MAE = Mean absolute error (Willmott, 1982).

MBE = Mean bias error (Willmott, 1982).

RMSE = Root mean square error.

RT = Model accuracy (Freese, 1960).

E\* = Five percent critical error as defined by Reynolds (1984).

GPSM = Grains per m2

LAI = Leaf Area Index

Parameters 1 through 7 were evaluated without using N routines (see Tables 3 and 4), whereas parameters 4 through 12 specially refer to aspects of the N routines to be tested (see Tables 1 and 2).

Table 3. Summary Measures for Data Sets Without N Routines

\_ \_ P = a + b\*0

Variable Unit n O P So Sp a b R d

Anthesis days 82 144.6 144.2 30.3 28.4 14.6 0.8960 0.912

Phys mat days 76 176.0 176.6 28.4 28.5 4.7 0.9763 0.947

Yield kg/ha 157 5,547.0 5,646.8 2,219.0 2,578.2 582.2 0.9166 0.633 0.88

Grain wt mg/kernel 144 38.3 36.4 9.3 9.4 13.4 0.6234 0.448

GPSM #/m2 138 14,594.6 15,161.2 5,115.2 5,811.9 5,507.3 0.6715 0.376

Dry matter g/m2 76 1,179.2 1,559.1 525.5 412.2 791.8 0.5052 0.411

LAI -- 54 4.4 5.2 2.6 1.6 3.3 0.4342 0.260

Table 4. Difference Measures for Data Sets Without N Routines

Max Min

Variable Unit n MBE MAE Error Error RMSEu

Anthesis days 82 -0.4 5.67 32.0 0. 8.5

Phys mat days 76 0.6 5.1 18.0 0. 6.6

Yield kg/ha 157 99.8 1,272.8 3,468.0 6. 1,552.0

Grain wt mg/kernel 144 -1.9 5.8 28.4 0. 6.5

GPSM #/m2 138 566.6 3,444.1 17,446.0 17. 4,437.5

Dry matter g/m2 76 379.9 352.0 1,324.0 2. 320.0

LAI -- 54 0.8 1.8 5.7 0. 1.9

## DATA BASE

Since model development and testing is an iterative process in the early stages, most of the data sets have been utilized during the development phase and are not truly independent. Since development of

CERES-Wheat-N has necessarily lagged behind the development of CERES-Wheat, the opportunity to rigorously test the model with a large base of truly independent data sets has not yet arisen. Development and testing of the CERES-Maize-N model (Jones and Kiniry, 1986) has paralleled the work on the wheat model. Because the soil N transformation components of both models are identical and since the basic structure of the CERES-Wheat model dictates the nature of biomass production, yield component determination, and water balance, the testing data base can be inferred as having a sufficient degree of independence from model development. Other data sets have been used extensively in model development and calibration which have not been included in the analysis.

To test the CERES-Wheat model under different growing conditions, a data base was assembled to represent a diversity of environments, including short growing season spring wheat crops, environments with limited water availability, sub-tropical wheat growing areas with little vernalization, and regions with temperature extremes. The data base represents a time span of 25 years (1959 - 1984) and a range of latitudes from 54o N (West Germany) to 36o S (Australia) (see Fig. 8.1). This includes published experimental data as well as unpublished dissertations and other unpublished sources.

Fig. 8.1. Location of experimental sites.

Because a complete minimum data set was rarely available, the additional climatic and soils information was obtained mainly through personal communication. When a few key data were unavailable, certain model inputs were estimated using the best available information and the approaches described in Chapter 5.

A good data set should contain as much detail as possible to describe the process of plant growth. However, taking a sufficient number of samplings throughout the season is time consuming and expensive and was therefore performed only in experiments especially laid out for model testing. These were particularly valuable, because results of such experiments allowed for the decription of the time course of several aspects of plant growth and comparison with model output.

For a detailed description of individual data sets see Otter-Nacke, Godwin, and Ritchie (1986).

## DIFFERENCE MEASURES AND SUMMARY STATISTICS

Phasic Development

The accuracy of simulating the phasic development of a crop is crucial for accurate simulation of crop growth and yield. Thus, evaluation of phasic development should be the first step. Observed and predicted means are close together with small RMSE, and similar standard deviations. While the intercept (a) is relatively close to zero and the slope (b) relatively close to unity for physiological maturity, this is not the case for anthesis date (see Tables 3 and 4).

Grain Yield and Components

Predicted yields versus observed yields are depicted in Fig. 8.2 and 8.3. Most predictions are within the limits of + 1.0 standard deviation. In only 30 out of 240 and 24 out of 157 cases, the difference between observed and predicted yield was larger than 1 standard deviation. Comparing the difference measure (d) for runs with and without account for N application summarizes the differences of all of these statistical parameters. D-values amount to 0.91 and 0.88, which indicates the model, including N- routines, is more accurate compared to runs without N routines. This is not a thorough test, however, because runs were performed on different data sets. CERES-Wheat tends to over predict yield. Means and standard deviations of predicted yields using or bypassing N routines approach those of the observations (Tables 1 and 3).

Fig. 8.2. Grain yield. Comparison of predictions of the CERES-WHEAT model with observed data from experiments.

\_\_\_\_\_ is the 1:1 line.

----- is the regression line between observed and predicted.

- - - Mark the boundary of + 1 standard deviation from the regression line.

Fig. 8.3 Predicted versus measured yield.

Kernel weight and grain number per m2 are the two composites of grain yield. Performance of the model in predicting these parameters was in general poorer than the simulation of grain yield. MBE indicates the model to over estimate grain weight under fertilized conditions (Table 2), whereas with N- routines switched off, the negative MBE suggests the contrary (Table 4). This is surprising because N is assumed to be non-limiting in the latter case. The intercepts and slopes of the corresponding regressions are likely to be significantly different from zero and unity (Tables 1 and 3).

This is also obvious for the regression of prediction on observed number of kernels per m2 without account for N effects (Fig. 8.4). Though the regression line is closer to the 1:1 line when testing N application data sets (Fig. 8.5) there is still considerable scatter outside the standard deviation limits. Error biases of kernel number and kernel weight are alternating, suggesting the two genetic parameters G1 and G2 (responsible for the determination of kernel number and kernel weight) being estimated poorly to accomodate data sets of different origin. MAE and RMSE are of similar value.

Fig. 8.4. Predicted versus measured number of grains.

Fig. 8.5. Grains /m\*\*2. Comparison of predictions of the CERES-WHEAT model with observed data from experiments.

\_\_\_\_\_ is the 1:1 line.

----- is the regression line between observed and predicted.

- - - Mark the boundary of + 1 standard deviation from the regression line.

Dry Matter and LAI

More scatter around the 1:1 line occurred for biomass predictions than for grain yield (Fig. 8.6 and 8.7). Means and standard deviations of predicted and observed dry matter differ more in data sets without account for N.

Fig. 8.6. Dry matter. Comparison of predictions of the CERES-WHEAT model with observed data from experiments.

\_\_\_\_\_ is the 1:1 line.

----- is the regression line between observed and predicted.

- - - Mark the boundary of + 1 standard deviation from the regression line.

Fig. 8.7. Predicted versus measured above ground dry matter.

MBEs are positive indicating a tendency to over predict dry matter production. Other coefficients show the model simulation is acceptable over a range of total dry matter yields from 448 to 3389 g/m2. The slope of the regression line for N trials (Fig. 8.6) supports the observation of over prediction. In the N non-limiting sets, the slope is only 0.5052 mainly due to a few outlyers at the high end of the range where dry matter was strongly under predicted.

Summary and difference measures only are given for leaf area index (LAI) (Table 3 and 4) because the error associated with measured values of LAI are usually very high. In this particular case, maximum LAI was requested for comparison between predicted and observed values. LAI measurements however, being time consuming, were not taken often enough to meet the peak of leaf area development. MBE being 0.8, indicates the model to over predict LAI by 18 percent on the average. Standard deviations are quite different, and intercept and slope are definitely different from zero and unity. These statistical values are not particularly meaningful, however, under the above premises.

Total N uptake, grain N uptake and grain protein values are of special interest when the nitrogen switch in the model is turned on. Simulation of these parameters is related to yield simulation, but did not excel as yield simulation. Forty-four points from a total of 223 fall outside the bounds of + 1.0 standard deviation of the 1:1 line for total N uptake (Fig. 8.8). For grain N uptake and grain protein percentage (Fig. 8.9 and 10) this was 31 from 215 and 60 from 215. Intercept and slope are just beyond the 5 percent confidence intervals, whereas other statistics suggest the simulations are acceptable. Total N uptake and grain N uptake were slightly over predicted.

Fig. 8.8. Predicted versus observed N uptake at maturity.

Fig. 8.9. Predicted versus observed grain N uptake.

Fig. 8.10. Predicted versus observed grain protein percentages.

Much of the error involved in simulation of total N uptake was related to poor simulation of N concentrations in the straw at harvest,

because grain N uptake was simulated fairly closely. Different harvesting techniques bear potential discrepancies, when e.g. substantial amounts of chaff or leaf material are included in the sample. The model does not account for losses of N through either leaching from harvest ripe straw or volatile losses from senescing leaves.

The scatter of points around the 1:1 line was higher for grain protein than for total and grain N uptake (Fig. 8.10). Only the modified Freese statistic indicates the model is still acceptable (Table 2). Simulation of grain protein content has been, to date, one of the most difficult components in the model. Determining whether a genetic factor controls some of the variation in grain N contents is difficult. Introduction of an additional genetic coefficient has so far been avoided.

For further details of the performance of aspects of the N routines see Godwin (1987).

## GRAIN YIELD RESPONSE TO SOWING CONDITIONS, IRRIGATION AND N APPLICATION

Sowing Density

Response curves to major input variables are a pictorial method to demonstrate the model's ability to react correctly to varying input. Sowing density is very common to vary with site or management system. Climatic conditions do not often allow for high densities, because stored soil water plus rainfall are not sufficient to support a large number of plants per unit area of land.

Lelystad is a site in the Netherlands where water is not a limiting factor. Performance of crops planted at densities ranging from five to 800 plants/m2 was compared focusing on the tillering process. In Fig. 8.11, observed and simulated yields in response to increasing sowing density are given, demonstrating that even for this environment the optimal sowing density is between 100 and 200 plants/m2.

Fig. 8.11 Lelystad 1977. Observed and simulated yields in response to increasing sowing density.

The model provides a very similar response. However, the difference between observed and simulated yields is 2238 kg/ha at the lowest sowing density of five plants/m2 and thus exceeds the + 1 standard deviation limit. In absolute terms this seems to be a large error. In the context of the entire experiment, however, it appears to be acceptable.

Irrigation

Comparisons of predicted and observed grain yields at 120 kg N/ha and different irrigation schedules are shown for three varieties at the arid wheat growing site, Tel Hadya in Syria (Fig. 8.12). Increasing fertilizer use with increasing amounts of irrigation was observed and also simulated. Varietal differences were higher in simulations than in reality. The model consistently over estimated N response in variety Sonalinka and the effect of none or little irrigation in variety Mexipak.

N Application

Out of a number of response curves of grain yield response to differing N application, Fig. 8.13 demonstrates the capability of the CERES-Wheat model to simulate location specific responses to N fertilizer application. Over a range of 0 to 210 kg N applied per ha, the model provided grain yields which were very close to measured yields at Rothamsted in 1975. The optimum application rate and differences between varieties were also reflected in these response curves.

In another location, Flevopolder, The Netherlands, no response was shown by the model for N rates ranging from 50 to 200 kg/ha, although a 25 percent increase in yield could be measured (Fig. 8.13b).

Fig. 8.12. Comparison of predicted and observed grain yields at differing fertilizer rates for three varieties with different irrigation strategies at Tel Hadya Syria, 1980.

Fig. 8.13. Comparison of predicted and observed response to applied N to the application pattern of N in individual data sets at Rothamsted, United Kingdom, 1975.

Fig. 8.13b. Comparison of predicted and observed response to applied N to the application pattern of N in individual data sets at Flevopolder, Netherlands, 1975.

The amount of fertilizer applied and the time of split application may result in different grain yields. For three locations, Lancelin (Western Australia), Bozeman (Montana), and Wageningen (Netherlands), simulated and observed yields are compared for five to seven different fertilizer strategies (Fig. 8.14). Response pattern was reflected well in model simulations. In cases where simulated yields did not coincide with observations, yield was over estimated at different degrees.

## SEASONAL PATTERN OF MODEL OUTPUT COMPARED TO OBSERVATIONS

Tracing the seasonal pattern of different aspects of plant growth, such as different plant parts, LAI or tiller development, and checking against real world observations is another way to locate errors in the simulation process thus ensuring accuracy. A few examples of experimental data used for this purpose follows.

Fig. 8.14. Comparison of predicted and observed grain yield response to differing fertilizer split application patterns.

Dry Matter

The seasonal pattern of dry matter has been checked intensively. A representative example for a very good match with data taken from a crop, which was managed like a farmer's field, comes from Weihenstephan, West Germany, 1983 (Fig. 8.15). Two contrasting varieties, Caribo and Maris Mardler, the latter being more adapted to a cool, humid climate, performed well and produced matching yields. The timing and amount of biomass production was in accord with observations.

Fig. 8.15. CERES-Wheat (non-nitrogen) model validation results from individual experiments; predicted versus observed at Weihenstephan, West Germany 1983.

Dry Matter Partitioning

Several experiments have been conducted to evaluate dry matter partitioning between plant parts over the course of the growing season, e.g. in Nottingham, 1975. Data from this experiment were compared to model values (Fig. 8.16). LAI and root weight were over estimated by the model resulting in slightly higher than observed total dry matter values. Partitioning plants into leafs, stems, and ears, which are sinks in different stages of the plant life cycle, illustrates which parts may not have been modelled satisfactorily. In this case, maximum predicted leaf weight was about 400 g per m2 higher than observed. This completely makes up for the amount of over estimated dry matter, because stem and ear weights were in perfect accord with observations in the experiment.

A different situation was found in a 1971 experiment in Rutherglen, Australia, where measurements were taken on a biweekly basis (Fig. 8.17). Ear weight was simulated well, but stem weights were missed considerably. This could be related to a different definition of plant parts, such as leaf sheaths being included either in the stem weight or leaf weight. The amount of assimilate partitioned to the roots was obviously too high over the whole growing season.

Leaf Area Index (LAI)

Fig. 8.18 compares model produced LAI values with observed LAI in an experiment in Roodeplaat, South Africa, where varying amounts of irrigation water was applied at different times. Plots receiving higher amounts of water (irrigations 3 and 5) produced denser canopies which could be simulated well. In irrigation 2 and 4, the timing of LAI build-

Fig. 8.16. CERES-Wheat (non-nitrogen) model validation results from individual experiments at Nottingham, England, 1975; predicted versus observed.

Fig. 8.16. Continued.

Fig. 8.17. CERES-Wheat (non-nitrogen) model validation results from individual experiments at Rutherglen, Australia, 1971; predicted versus observed.

Fig. 8.17. Continued.

Fig. 8.18. CERES-Wheat (non-nitrogen) model validation results from individual experiments at Roodeplaat, South Africa, 1978; predicted versus observed.

Fig. 8.18. Continued.

up was correct, but LAI was small. Irrigation 1 resulted in a different model leaf area development, where the timing was later than observed in the field and maximum LAI was close to 4 rather than 2.5 as measured in the experiment.

Tiller Development

Modeling tiller development satisfactorily has been one of the more difficult tasks, because this process is controlled by a set of environmental, inter- and intra-plant conditions. The effect of sowing density on tiller development under arid conditions was monitored in a 1984 experiment in Temple, Texas (Fig. 8.19). The normal shape of a tillering curve was observed at the common sowing density of 160 plants/m2 and the model was able to simulate this curve perfectly. At 40 plants/m2 the model missed the peak of tiller development observed in the field at ca. 1200 tillers/m2. In the lowest sowing density of 10 plants/m2 the model maintained the number of tillers built early in the season until harvest, whereas some degree of tiller abortion was observed in the field.

The first measurement in the highest density plot was taken about 90 days after sowing when the tiller number for this dense crop was at maximum and some plants had up to 40 tillers. Some error could be associated with the sampling technique so that missing this data point is not considered to be crucial. For the rest of the season there was good agreement between modelled and observed tillers with the final number of tillers being correct.

Fig. 8.19. CERES-Wheat (non-nitrogen) model validation results from individual experiments at Temple, Texas, 1984; predicted versus observed.

## CONCLUSIONS

The CERES-Wheat model is designed to be used as a management-oriented simulation model for a diversity of applications in all environments suitable for wheat growing. To make the model useful to an audience as wide as possible, the inputs must be minimal and they must be reasonably easy to attain or estimate from standard agricultural practice. Under these premises, the model simulates crop growth and development, response to N fertilizer, irrigation, sowing time and density reasonably reliably. Rigorous statistical analysis indicated acceptance of model simulations. However, some problems have yet to be resolved with the prediction of tiller development, N uptake and grain protein concentration as suggested by comparison with a few data sets. A slight tendency to over predict biomass and N uptake early in the season was noted. Further data sets are required to test more rigorously the soil N components of the model. Additional testing and refinement of the indicated parts of the model may be beneficial.

# CHAPTER 9

# KNOWLEDGE GAPS

The nitrogen components of the model have been constructed with the philosophy of maintaining simplicity and a state of balance with the remainder of the model. The model itself has been constructed within the framework of keeping the number of inputs required to a minimum and to those which are easily attainable. This latter constraint has generally precluded the use of laboratory procedures to characterize soil and site specific rate constants for the nitrogen transformations. In some instances predictions would undoubtedly be improved if appropriate specific rate constants were used as inputs, but this would detract from the generality of the model. Methods of estimating these rate coefficients from other more commonly available soil properties are needed if improvement in the predicted rates of the various transformations is to be made.

The CERES model does not simulate losses of nitrogen via ammonia volatilization. While arguments can be made that under conditions of good fertilizer management (placement of fertilizer especially) these losses should be small, there are conditions where losses can become substantial. Ammonia loss from surface applications of urea to alcareous soil and from anhydrous ammonia bands can be large. Several models exist within the literature to simulate these losses (eg. Rachhpal-Singh and Nye,1986 and McInnes et al) but all operate at levels of detail beyond that used in CERES. A simple method of predicting ammonia loss that requires only modest inputs is sorely needed. Among the factors known to be important are soil moisture content, soil pH, soil cation exchange capacity, temperature and soil hydrogen and ammonium ion buffering capacities.

The procedures to describe leaching of nitrate within the model are very simplistic and as pointed out in some circumstances may be inadequate. Addiscott (1981) has described a model that partitions water and solutes between a mobile phase and a retained phase. The partitioning was made on the basis of a two bar moisture content. The CERES model does perform some partitioning of the moving water on the basis of the whole profile saturated water conductivity (SWCON) and also on the partitioning between water below the drained upper limit and above it. Appropriate procedures to enable the partitioning of nitrate between these various soil water phases are required. The procedures would need to account for differences in equilibration of solute between these phases which would occur in different soils.

One problem encountered with the nitrogen components of the model was the inability to accurately predict mineralization of nitrogen on certain unusual soils. The model under predicted the mineralization rate on virgin soils which have been recently cultivated. In other instances where "protected" organic matter occurs in some andosols the model over predicts mineralization. Currently provision is made to adjust the mineralization rate with an arbitrary user-supplied scalar DMOD for these circumstances. An appropriate way of identifying these circumstances or adjusting the mineralization rate constant (DMINR) for these soils is required. Laboratory procedures (eg Stanford et al 1972) exist for this, but the estimates are not commonly available. A surrogate value which could be estimated from other soil properties may be possible. Another problem which exists with the mineralization calculations is concerned with determining the appropriate way to initialize the fresh organic matter pools. These are currently initialized as 20% carbohydrate, 70% cellulose and 10% lignin.

When fertilizer is placed in a band or point placed, the model assumes uniform incorporation within the layer in which the fertilizer is placed. When high concentrations of fertilizer affect the chemistry of the soil in such a way as to substantially alter the nitrogen transformation rates this simplification will be in error. These fertilizer practices are of more concern in wide-row crops and should not greatly affect the simulation of nitrogen dynamics in wheat cropping systems.

One significant problem encountered when attempting to simulate the accumulation of nitrogen in the grain was how to account for genotypic differences in grain protein accumulation. The model in general terms can account for differences in temperature, soil water status, and plant N status on grain N accumulation. However, the simulations are often poor. Several researchers have pointed to cultivaral differences (Hunt 1984). A further genetic coefficient describing the rate of grain N accumulation per degree day or alternatively some factor defining cultivaral differences in the minimum vegetative N concentration during grain filling is probably required. Cultivaral differences also occur in the critical concentration growth stage relationships. However, other than differentiating between winter and spring wheat cultivars, no attempt has been made to separate these out.

In some experiments nitrogen has been reported to have an effect on growth duration of the crop. Often high nitrogen treatments are reported as having a delayed maturity. One possibility for this is that under a higher plane of nutrition tiller survival is greater. Since anthesis and maturity on higher order tillers are later than on the main stem, the mean anthesis and maturity date for the whole plant are delayed. An alternative hypothesis advanced by Davidson and Campbell (1982) is that the increased canopy growth associated a higher N rate in some way may contribute to a cooler meristem either through greater shading or via greater transpiration. Further research is needed to determine the mechanisms of this delay before it can be modelled.

# CHAPTER 10

# MODEL APPLICATIONS

Several research groups have developed crop models to evaluate various aspects of the crop system. This chapter will be a brief overview of the various applications of those models.

## MANAGEMENT AND CROPPING STRATEGIES

Alocilja and Ritchie (1988) developed a software package for agricultural extension workers, researchers and government policy makers to use in the design and management of the rice-production system. Using the CERES-Rice model in conjunction with the simulation multicriteria optimization technique (SMOT), these individuals can be assisted in decision making for agrotechnology transfer.

Using data from South Africa, deVos and Mallet (198-) evaluated CERES-Maize and CORNF for assessing cropping strategies. They found that the models agree well with observed values of total above-ground plant dry mass, leaf area index, grain yield and soil water content. They also found that CORNF tended to underpredict leaf area index, and CERES-Maize provided realistic estimations of soil water content.

## PREDICTING YIELD

"Tom Hodges (University of Missouri), S.K. Leduc (NOAA/NESDIS) and A. Eddy (Oklahom Climate Survey) used the CERES-Maize model to forecast yields during the 1983 drought. The researchers used actual weather conditions up to July 1, but simulated the weather for the remainder of the growing season based on historical data. The model was run at 51 first order stations in 14 midwestern states.

Hodges et al. (1987) tested the ability of CERES-Maize to predict annual fluctuations in maize (zea mays L.) production in the U.S. cornbelt for a four-year period, 1982-85. Results indicate the model may be used for large area yield and production estimation in the U.S. with minimal regional calibration. It also has potential for large area yield estimation in other parts of the world where daily maximum and minimum temperature, precipitation and solar radiation data are available.

Botner et al. (1986) also used CERES-Maize in projecting corn yield in the U.S. cornbelt. Test results indicate that using simulation models in an operational context for large-scale crop yield estimation is feasible and can be accomplished within reasonable cost if historic data and calibrated inputs to the model parameters have been determined.

Fei, Qing-Pei and Ripley (1985) used the CERES-Wheat model in southern Saskatchewan as an operational tool to predict yields. They initially tested the model with 25 years of historical data from the Saskatoon crop district. After correcting for a "technology trend" of 32 Kg/ha per year, they found that the CERES model was capable of simulating yields for 1960-84 with a correlation coefficient of 0.70. They also found that the main weakness in the model is over estimation in high yield years and under-estimation in low-yield years. This problem appears to be caused by the model's inability to simulate adequate root growth.

Larsen (1981) worked with CERES-Wheat and TAMW to determine whether a plant growth simulation approach could be successfully used to make large-area yield forecasts for winter wheat. Results showed that many plant responses are simulated well but improvement is needed in several areas before accurate yield forecasts can be realized.

"A. Van Dyk and Tom Hodges (University of Missouri) used CERES-Maize in a study that linked satellite information with crop simulation models. The study utilized satellite data to provide inputs on leaf area index, solar radiation, and crop emergence. Actual yields were compared to yields produced by CERES-Maize.

"W.R. Berti, D.L. Karlen and J.E. Pasons (all USDA-ARS, Florence, SC) used CERES-Maize to compare measured and predicted corn yields as affected by soil series. Results indicate that predicted values on corn grain yields ranged from 95% to 19% greater than measured values for six soil types included in this study. They recommend that site-specific data on initial soil water and depth of rooting could be used to improve predictions.

"E.L. Piper and A. Weiss (both University of Nebraska) are evaluating the response of a structured version of CERES-Maize to reduction in plant population or defoliation at various life stages. CERES-Maize projections were as much as 38% less than actual results when the population was reduced during vegetative growth. The model over-predicted kernel number and under-predicted kernel weight, except at 100% defoliation during vegetative growth. The authors suggest that the relationship between carbon redistribution during vegetative growth after defoliation, and the prediction of kernel number should be investigated.

"William Iwig and Benjamin Klugh, Jr. (both USDA Statistical Reporting Service, Washington, D.C.) have evaluated two feedback versions of the CERES-model. The first version forces the modeled values of leaf number and vegetative biomass to statistically match measurements of the observed corn crop made on any day prior to tasseling. The second version performs additional adjustments to the modeled yield components of kernels per plant and kernel weight based on feedback data. Analyses using six test data sets indicated that only the second feedback version produced significantly improved estimates of yield and kernel weight, and that neither version produced improved estimates of kernels per plant.

"Keating, et. al, have been adapting the CERES-Maize model for use in eastern Kenya where rainfall is low and unreliable. CERES-Maize was used to examine the effects of plant population on the long-term returns and risks of maize production at two sites in Kenya with different levels of soil fertility. Results indicate that high plant population would tend to increase long-term average yields in areas with non-limiting soil fertility. However, where nitrogen is strongly limiting, high plant populations were expected to reduce long-term average yields and increase the risks of crop failure. The model provided an accurate description of grain yield, but simulation of above ground biomass was less accurate."

"Carberry, et al. have been validating CERES-Maize in semi-arid, tropical environments in Australia, and have been adapting it for use in such areas. The model initially did not predict yields accurately in the Northern Territory region of australia. Functions of the model describing phenology, leaf growth and senescence, and grain growth were later revised and validated. Subsequent calibration reduced the root mean square deviation for observed grain yields from 3480 to 2015 kg/ha."

"Mulliken has reported successful results in using the CERES-Maize model to predict yields. Mulliken reported that the model predicted 116 bushels per acre (bu/a) for a dryland corn crop and the actual yield was 113 bu/a. In another instance where the corn was irrigated, CERES-Maize predicted yields of 198 bu/a and actual yields were 194 bu/a.

## PREDICTING CLIMATE IMPACTS ON GROWTH AND YIELD

"A.L. duPisani used CERES-Maize as a drought prediction tool. The model is being used to assess drought impacts on maize at an early stage so that policy makers can have an objective measure to declare drought-stricken areas. To assess the impact of early season weather on crop yields, the model was run with actual weather data up to a given date. Historic data were used for the remainder of the growing season. Excellent correlations were found between yield predictions and actual yields."

## DROUGHT INDEXING

Booysen (1987) used wheat growth simulation models (the CERES model, Ritchie 1985; the Utah model; the Kanemasu model, Kanemasu, et al.; and TAMW) to determine their effectiveness in deriving a crop specific drought index (CSDI). Featuring the environment and the crop, i.e. transpiration, root absorption, phenological growth stages, and the climatic and soil moisture variables, the CSDI performed better than the Palmer drought severity index by a small margin. A simpler empirical model may have achieved the same results as the more complex models, but calibration and adaptation to the area would most likely have had to be performed.

## IRRIGATION

Algozin (1986) used CERES-Maize to identify irrigation scheduling strategies for efficient use of natural resources and for economic profitability. His results show that economic efficiency was achieved at high application rates while irrigation water productivity was highest at small application rates.

Berrada (1983) used the CERES-Wheat model to study continuous wheat and fallow-wheat cropping systems and then compared no-till and conventional tillage within each system. Higher yields and lower incidence of failure were achieved with no-till than with conventional tillage in continuous wheat. In fallow wheat however, these two tillage methods performed similarly. According to Berrada, the simulation results confirm the hypothesis that with a no-till management system, continuous winter wheat can be a feasible alternative to fallow-wheat in western Nebraska.

Worman et al. used the CERES-Maize model to compare dryland and fallow cropping and various levels of irrigation. The model was validated by simulating yields for field experiments performed over an 8-year period. They found the simulated yields were close to actual yields.

"Boggess and Ritchie used CERES-Maize to link agronomic crop response information with economic and financial data in economic analysis and risk assessment of alternative irrigation strategies. CERES-Maize was used to generate yield predictions and alternative irrigation strategies. Alternate irrigation strategies were ranked on the basis of net returns and risk. Boggess summarized that the optimum management strategy depends on whether the producer desires to maximize yields, profits, or utility."

## DRAINAGE

Brink (1985) linked a CERES crop model with a water management model DRAINMOD and created a model that simulates crop growth and yield as well as handles water balance for a water management system. A better description of the effective root zone depth was achieved because the roots responded realistically to soil water conditions existing in drainage. Also, by adding a supplementary method that accounts for the presence of a water table, he obtained an improved evapotranspiration routine.

## WATER FLOW AND SOLUTE TRANSPORT

"K.W. Molten, J.C. Parker, T.B. Brumback, J.C. Baker and E.W. Carson (all of Virginia Tech University) have developed an enhanced version of CERES-Maize by adding an adapted version of the RHIZOS portion of the cotton growth model GOSSYM. RHIZOS uses a two-dimensional transport approach to simulate the movement of soil water and nitrate. The enhanced model allows the user to select a water balance or a two-dimensional transport approach to the movement and plant uptake of water and nitrogen."

## NITROGEN UPTAKE

"Jones and Kiniry evaluated the performance of the CERES-Maize model from several locations and disciplines over the past six years. Model predictions were compared with measured values for experimental data from many regions. The nitrogen-limiting version of the model produced realistic simulations of the effects of nitrogen on biomass, total nitrogen uptake, grain nitrogen concentrations, total nitrogen in the grain and grain yield. The non-nitrogen version produced estimates of maximum leaf area index, maximum above ground biomass grain numbers, and grain yields which had highly significant correlations with measured values."

## FERTILIZER

"C.A. Baanante, D.C. Godwin and J.T. Ritchie used the CERES-Maize and CERES-Wheat models coupled with a stochastic weather generator to simulate responses to various fertilizer strategies in Australia and Benin, West Africa. For each strategy, 50 crops were simulated. Strategies were compared on the basis of yield, total added return, and net benefits of fertilizer. Results indicated substantial differences between strategies in Benin, but only small benefits in Australia. Godwin and Ritchie also tested the sensitivity of the nitrogen component of the CERES-Maize model by two methods. First, 1-year field experiments were simulated and the impact of changing nitrogen management variable (fertilizer rate, timing placement, depth, and source on yield and nitrogen uptake) was examined. Second, climatic data were used to simulate the growth of 50 crops. analyses indicated CERES-Maize exhibited high sensitivity to climatic variables and some soil variables, but less sensitivity to nitrogen transformation rate variables.

## ROOT GROWTH

Bland (monograph chapter) and Jones, Bland, Ritchie and Williams (monograph chapter) used models to simulate root system growth. The models flexibility and responsiveness enabled them to simulate root growth in a variety of soils, climates and species, and generated root length density profiles similar to those documented in the literature.

## PEST MODELING

Muchen (Ph.D. thesis, 988) used the CERES-Maize model to learn more about the ecology and management of a major nematode pest(Pratylenchus Zeae) of maize in Zimbabwe. The model predicted the population density of P. Zeae in maize roots with a mere error of 7%; it was sensitive to weather data and to different initial population densities of P. Zeae in the soil; it predicted the correct silking date of maize variety R215 and above- and below-ground dry biomass with mean errors of 17.7% and 11.1%. The research showed the model could be incorporated in future predictive P. Zeae maize yield and crop loss assessments.