SIMULATION MODEL FOR PLANT GROWTH
IN CONTROLLED ENVIRONMENT SYSTEMS

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INTRODUCTION

Among the requirements for a self-sustaining regenerative CELSS are atmospheric regeneration by reduction of carbon dioxide and evolution of oxygen and reincorporation of the reduced carbon into the organic constituents of human food. A controlled-environment crop production system is a probable component in accomplishing these requirements. However, higher plants, together with their reactions to environmental and cultural conditions, comprise an extremely complex biological system, and inclusion of a crop production system in a CELSS requires answers to questions of its reliability and predictability to meet the regenerative requirements in response to perturbations in the environmental conditions and its flexibility for controlled levels of functioning in optimization of mass flows within a CELSS in response to selected environmental conditions. Two concerns in evaluation of crop reactions to environmental conditions are how to evaluate effects of environmental conditions on crop growth and yield, and once any set of environmental conditions has been experienced by the crop, what can be done to readjust crop growth and yield to levels for optimization of the CELSS. The capability to respond to the latter concern depends on the ability to evaluate probable outcomes of possible management strategies, including selections from among available environmental conditions. Mathematical modeling of the crop system can assist in addressing these questions and in interpreting the results of discrete experimental studies of crop reactions to environmental conditions.

The crop system that must be addressed is one of a community of plants growing under conditions selected by management and by possible malfunctions. But the complexity of the system makes it inherently difficult to define. The complexity of the crop production system is manifested in the large number of interacting variables needed to describe the inner workings of the system, in the large number of possible behavioral responses and in the large number of environmental regimes to which the system might be subject. Moreover, while the system itself can be highly complex, discrete experiments designed to provide information about the behavior of the system can be only as complex as will allow interpretation. In this context, then, the problem of evaluating the behaviors of crop production systems as a component of a CELSS is how to use a finite and relatively small number of experimental observations, made under relatively simple defined conditions, to make inferences to a nearly infinite set of possible conditions for a vastly more complex system.

THE ABSTRACTION HIERARCHY

In addressing the problems of a crop production system within a CELSS, it is useful to draw on the concept of abstraction hierarchy (Mesarovic et al., 1970) in which the levels of hierarchy refer to how coarsely or finely ground the system is taken to be. The following levels might be identified: (a) CELSS crop ecosystem level; (b) plant community level; (c) single plant level; (d) organ structures and elementary functional processes such as photosynthesis, respiration, translocation, etc., (e) elementary structures such as cells, membranes, local structured processes, etc.; (f) molecular physiology and chemistry; and (g) atomic and molecular physics. Each of these levels is meant to stand for a collection of subsystems or components that co-exist and

possibly interact within the level, and the next higher (coarser) level can be viewed as a level of organizational structure of these components (Gold and Raper, 1983). If one proceeds within the hierarchy from bottom to top, or finer to coarser levels, it becomes increasingly more difficult to control the experimental environment of the system. The breakpoint in biological systems comes at about the single plant level, for which it is possible to control the environment within phytotron and growth chamber facilities. (A phytotron is defined as an assemblage of controlled-environment chambers and glasshouses used simultaneously and in various combinations to investigate plant responses to environment, and the term thus implies function rather than size of the controlled-environment facility.) Thus, while inferences from experiments are desired for CELSS at least at the plant community level, or possibly higher at the crop ecosystem level, the observational level at which experimental conditions can be controlled is limited to that of single plants or very small groups of plants. The processes, such as photosynthesis, respiration, and translocation, that give rise to these observations and upon which extrapolation to higher levels must be based, are at yet a finer level. The ability to make inferences about the class of systems at the complex level of organization is, therefore, dependent upon the ability to draw relationships across levels in the hierarchy. Since the hierarchial structure is an artifact to facilitate scientific description of the system, the usefulness of such a description hinges on the ability to describe each of the levels and each of the subsystems at a given level independently of the other levels and subsystems.

As one proceeds up the hierarchy, it should be noted that the detail necessary to describe a lower level is specifically not wanted for the

description of a higher level (Gold and Raper, 1983). For example, consider the relationship between each component molecule and the aggregate content of carbon dioxide gas within the crop production system. Each of the $6.02 \cdot 10^{23}$ individual molecules within a mole of gaseous carbon dioxide are characterized by their individual positions and energy levels at any instant. While the extent of this clearly is more than one particularly wants to deal with for an aggregate description, the total collection of carbon dioxide molecules can be characterized by definition of volume, temperature and pressure. While these three variables that describe the high level are functions of the infinitely more extensive collection of variables that describe the lower, these functions have no inverse and informational detail is lost as one moves from a finer to a coarser level within the hierarchy. One role of a mathematical model of the crop system thus is to assist in expressing the relevant information functions and determining what detail needs to be retained to characterize the plant growth within the system.

While the behavior of a system at a higher level of abstraction is a function of behavior at the lower level, the lower level operates under constraints imposed by the organizational structure of the higher level (Mesarovic et al., 1970). In a biological system there is the additional complication that part of the behavior of the system at any level is to alter its own structure to cause a feedback relation between constraints and processes. An example of such an interlevel dependency is the rate of photosynthetic assimilation of energy by the plant. The leaf structure of the plant imposes a higher level on the interception and absorption of radiant energy as the input for the photosynthetic process during a time interval. During the time interval the

structure changes in response to the production of photoassimilates available for growth.

Several implications can be drawn from these general arguments about the relationship between levels of the hierarchial structure (Gold and Raper, 1983). First, interactions between subsystems at the same level tend to proceed through the interaction of lower level component processes such as the interaction between a plant and the aerial environment. The processes of carbon dioxide movement within and between the two components is governed by the constraints on molecular movement within each component and the structural relation between the two (which is a constraint imposed by yet a higher level of organization). Second, subsystems at different levels tend to operate on different time scales since changes at one level are functions of processes at the lower level. As an extreme example, consider morphological features, such as the position of leaves which are developed on a relatively long time scale of days and remain constant over even longer periods of weeks once built into the growth of a plant, and physiological characteristics, such as photosynthetic rate per unit leaf area, which are reversible on a relatively short time scale of minutes or seconds. Thirdly, an observation of the state of the system intrinsically involves an interaction between the system itself and the measuring device and involves processes at a lower level leading up to the observation. For example, attaching a plexiglas cuvette to a leaf to measure net photosynthetic rate by infrared gas analysis alters the microenvironment of the leaf, and the net exchange of carbon dioxide between the cuvette environment and the chloroplasts within leaf cells involves changes in thermodynamic constraints imposed by size and energy fluxes of the cuvette. Finally, because of feedback loops in

biological systems involving process functions (such as photosynthesis) and structural functions (such as leaf development) between levels and the absence of total cognizance of processes within any level, interlevel relationships cannot be derived from extrapolation from one level to another. Rather, interlevel relationships must be derived from interpolation between levels based upon an understanding of the physical laws that govern behavior of the system at the different levels and upon an understanding of the interlevel interactions.

SIMULATION MODEL FOR CROP PLANTS

Describing the dynamic relationships between levels of the system hierarchy is one of the functions of a mathematical simulation model of crop plants. Most crop simulation models are based on models for single plants, sometimes as modified by the presence of other plants. These models express growth and metabolic activity as a function of environmental variables, using mathematical forms suggested by knowledge of basic biochemistry and plant physiology. Verifying the applicability of these mathematical descriptions and determining values of the parameters to use generally required replicated experimentation under as carefully controlled and precisely identified conditions as possible. The conditions for these experiments should not be chosen for the purpose of direct extrapolation of results to a crop production system for CELSS, such as identifying a set of environmental conditions for maximum yield of a crop species. Although such studies are useful in defining the upper limits of productivity for the crop production system, sustained levels of maximum growth and yield do not optimize the entire CELSS. Also, the technology of ground-based experimental systems is likely not to be directly applicable to an

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actual CELSS. Rather, conditions for experimentation should be chosen for the purpose of verifying the mathematical formulation of the underlying plant physiology, for the purpose of testing the formulation of how the levels relate to each other, and for the purpose of learning the values of the appropriate parameters (Gold and Raper, 1983).

As an example of model development to relate individual processes to environmental conditions and behavior of the whole plant with possible application to CELSS, consider the simple, deterministic model for plant growth that we are working on at North Carolina State University. A mathematical simulation model is necessarily a simplification of the actual system under consideration in which essential characteristics of the actual system should be mimicked by the model. In this case our objective is to take into account the dominant features of plant physiology to describe plant growth subject to a wide range of variations in environmental conditions.

A general description of the model can be given without going into the mathematical detail (Wann et al., 1978, 1979, 1984). The effects of incident photosynthetically active radiation and ambient carbon dioxide concentration are incorporated directly through the process of photosynthesis and the effects of temperature directly through the processes of photosynthesis, respiration, growth, and aging. Leaves, stems, and roots are defined as separate organ classes during vegetative growth (Figure 1). For each of these classes, compartments are identified for soluble carbohydrate pool, young tissues capable of active growth, mature tissues incapable of active growth but otherwise capable of normal physiological functioning, growth
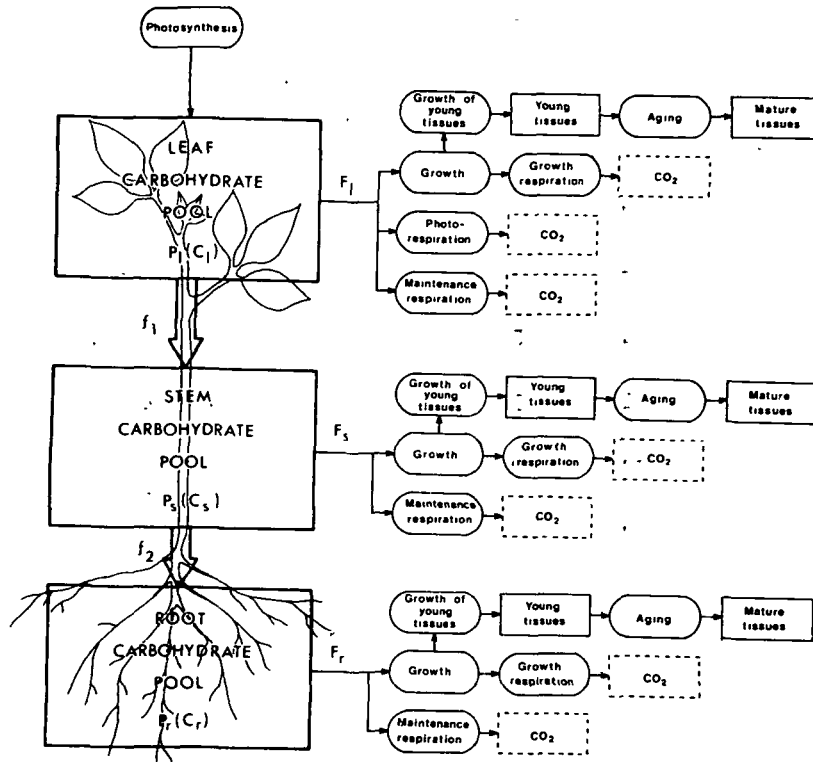
Figure 1. Energy and carbon flows in the plant system as adapted from
Wann et al., (1978, 1979, 1984, 1986). Rectangular boxes with solid
outline represent compartments within the plant system, rectangular
boxes with dashed outline represent compartments external to the plant
system, and elliptical boxes represent processes.

and maintenance respiration. An additional compartment for photorespiration

is identified for the leaves. Photosynthesis serves as the sole source for the

carbohydrate pool in the leaves, and net movement of carbohydrate is from the

leaf pool to the stem pool and from the stem pool to the root pool. Since

translocation fluxes between pools must be sufficient to maintain a living

state and to support normal growth of the organs, they are determined under two possible conditions (Wann and Raper, 1986). First, when carbohydrate supply in the source (exporting) organ is not limiting, the flux is assumed to be determined by demand of the sink (receiving) organ and by the availability of carbohydrate in the source pool. Source strength is considered as proportionate to the concentration of carbohydrate in the pool of the exporting organ and sink demand is defined as the amount of actively growing tissue in the receiving organ. Conversely, if carbohydrate availability in pools is insufficient to satisfy all demands of growth and respiration by organs, maintenance respiration and growth are assigned the first and second highest priorities for allocation of carbohydrate within the organ pool. The remaining carbohydrate in the source pool is then available for translocation to the sink organ.

Of the five classes of parameters included in the model, only four (the maximum photosynthetic rate, the specific respiration rates, the specific aging rates, and the maximum specific growth rates) are directly dependent on temperature (Wann et al., 1978, 1979, 1984). The fifth class of parameter, the translocation coefficients, are considered to be responsive to temperature indirectly through the effects of temperature on the concentration of carbohydrate in the source pool and the size and metabolic activity of the sink organ (Wann and Raper, 1984).

A set of nonlinear, ordinary differential equations (Wann et al., 1978, 1979) is used to describe the flow of energy (and carbon) through all compartments specified in Figure 1. For a given instant the net flow rates

for each compartment are computed as the difference between input and output flow rates. The entire set of differential equations has simultaneous solution to give a continuous simulation of plant physiological processes. Since the simulation of plant growth is continuous, the distinct conditions of pool sizes, average age of tissues, and metabolic activity that are reflective of the environmental history of the plant do not require updating at discrete intervals of time or growth stage, but are predicted by the performance of the model in response to environmental conditions during growth. Furthermore, this is the only simulation model for growth of the whole plant of which we are aware (Legg, 1981) that the effects of environment are incorporated mechanistically through their efforts on the processes of photosynthesis and respiration.

MODEL VALIDATION

Many of the important parameters required by the model, such as translocation coefficients and aging rates, are difficult to measure directly and can only be estimated by fitting the model against experimental data through the use of numerical integration and iterative weighted least squares techniques. Data initially used in fitting the model were obtained from experiments conducted with tobacco plants (Nicotiana tabacum L. 'NC 2326') grown for 35 days at constant temperature conditons over a range of 14 to 34°C and a constant photosynthetically active reaiation of 750 µmol m^{-2}s^{-1} in growth rooms of the phytotron at North Carolina State University. Plants were sampled at 2 to 3 day intervals during the growth period. The fit of the model was verified by comparing the dry weights of leaves, stems, and roots with the measured dry weights at each sampling date for each temperature (Wann et al., 1978).

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The model was then validated against independently derived data sets from experiments with natural variation in radiation under fixed temperatures in controlled-temperature glasshouses of the phytotron (Wann et al., 1978) and from experiments with weekly (Figure 2) and daily changes in temperature under constant radiation in growth chambers (Wann and Raper, 1984). The plants in all programs of weekly temperature change (Figure 2, inserts) were subjected to each of the five day/night temperatures during 1 week of the 5-week growth period, but since the sequence of temperatures was different in each of the ten programs, the plants in each of the programs experienced any single day/night temperature at a different combination of growth stage and previous temperature history. When reacting to a given temperature, the plants thus would be expected to have distinct conditions of pool sizes, average age of tissues, and metabolic activity. These factors are not updated at discrete intervals of time or growth stage for the continuous simulation of plant growth by this model, but reflect the performance of the model. Thus, the generally good agreement between predicted and measured performance of plants to changes in temperature (Figure 2) and radiation (Wann et al., 1978) indicates that the model is capable of responding to variable conditions during plant development.

Although the model was originally developed and validated with experimental data and parameter values for tobacco, it has been adapted for simulation of vegetative growth of soybean (Glycine max (L.) Merr. 'Ransom') with limited modification of parameter values and validated against data sets for plants grown in phototron chambers over a 28-day period at temperatures over the range of 14 to $34^{o}C$ (Figure 3) and for plants grown in hydroponic culture with independently varied root and shoot temperatures (Figure 4). The good

Figure 2. Simulated (continuous line) and measured (o) dry weights of
tobacco plants grown under the weekly changes in temperature schedules
shown in insets. Within the insets, the 9-h day temperature is indicated
by the continuous line and the 15-h night temperature is indicated by
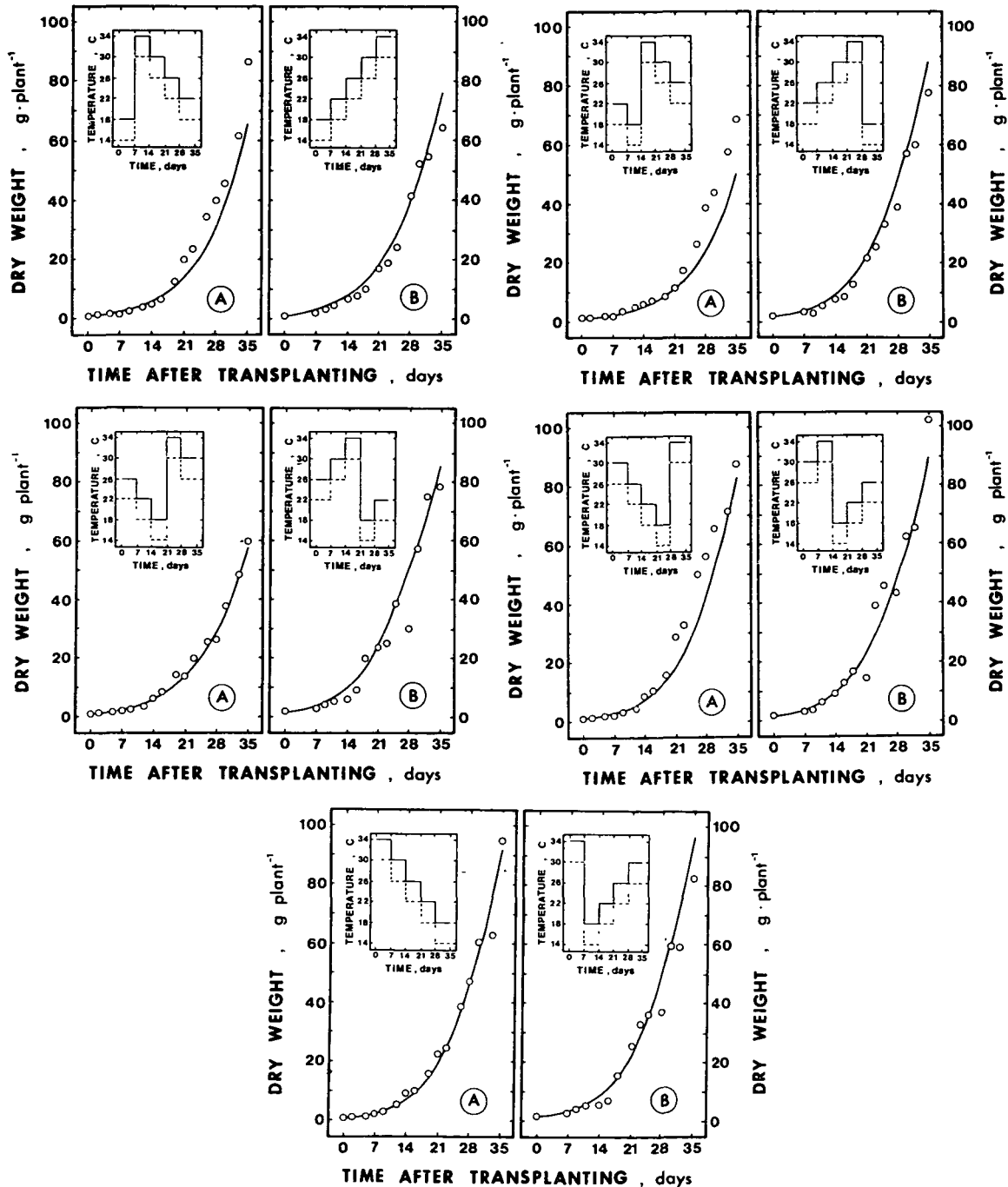the dashed line. (Adapted from Wann and Raper, 1984.)

Figure 3. Comparison of calculated and measured dry weights of soybean plants and plant parts under five constant day/night temperatures. Photosynthetic photon flux density during the 9-h day period was $750 \ \mu mol \ s^{-1} \ m^{-2}$. (Adapted from Wann and Raper, 1979.)
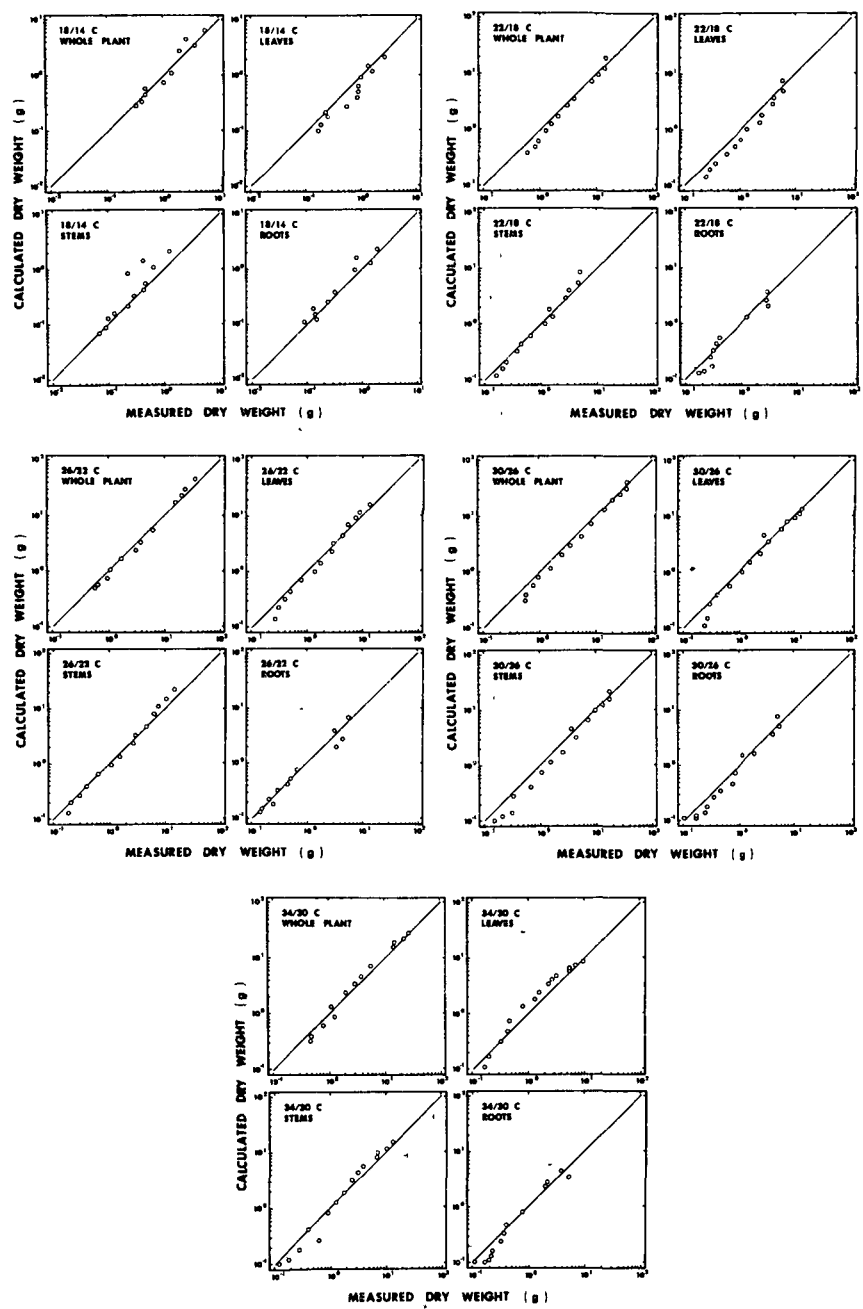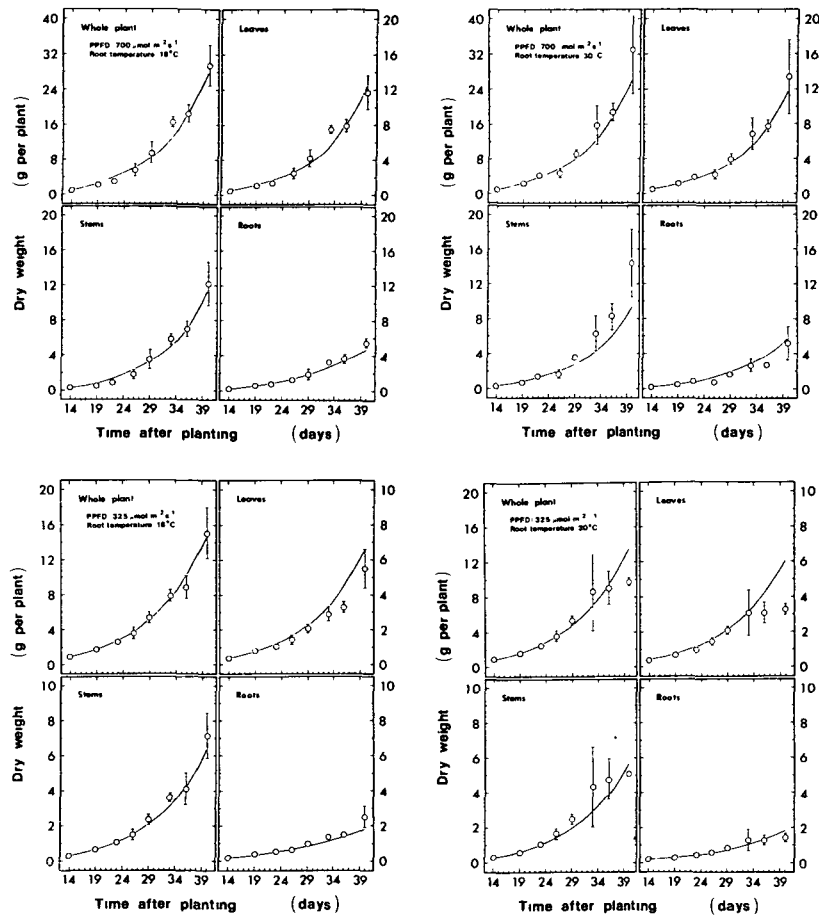
Figure 4. Simulated (continuous line) and measured (o) dry weights of soybean plants and plant parts grown in hydroponic culture at root-zone temperatures of 18 and $30^{O}C$ and photosynthetic photon flux densities of 700 and 325 μmol s^{-1} m^{-2} during a 9-h day period. Day/night aerial temperatures were $26/22^{O}C$.

agreement between predictions by the model and measured performance of two species of plants to perturbations in temperature and radiation indicates that the model structure is relevant to actual growth and can serve as a general model for growth of whole plants.

SUMMARY

The role of the mathematical model is to relate the individual processes to environmental conditions and the behavior of the whole plant. Using the controlled-environment facilities of the phytotron at North Carolina State University for experimentation at the whole-plant level and methods for handling complex models, we have developed a plant growth model to describe the relationships between hierarchial levels of the crop production system. The fundamental processes that are considered are (a) interception of photosynthetically active radiation by leaves, (b) absorption of photosynthetically active radiation, (c) photosynthetic transformation of absorbed radiation into chemical energy of carbon bonding in solube carbohydrates in the leaves, (d) translocation between carbohydrate pools in leaves, stems, and roots, (e) flow of energy from carbohydrate pools for respiration, (f) flow from carbohydrate pools for growth, and (g) aging of tissues. These processes are described at the level of organ structure and of elementary function processes. The driving variables of incident photosynthetically active radiation and ambient temperature as inputs pertain to characterization at the whole-plant level. The output of the model is accumulated dry matter partitioned among leaves, stems, and roots; thus, the elementary processes clearly operate under the constraints of the plant structure which is itself the output of the model. The values of those parameters,

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such as rate constants for respiration, growth, etc., that cannot be
directly measured as they operate in the intact plant but are necessary
for mathematical description of the elementary processes are inferred
from estimation procedures based solely on observations at the whole-
plant level under the controlled and repeatable experimental conditions
of the phytotron. The structure of the model thus provides the capacity
for interpolating among the levels within a crop production system of
a CELSS. Continuing development is being directed toward including
nitrogen nutrition and carbon dioxide as inputs to the model, extending
the structure of the model to include reproductive growth, and adapting
the model to run on a micro-computer.

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