(including an equation of ecosystem biomass dynamics) has shown that, due to nonlinear interconnections in this set, its behavior may be more complex (e.g., the integrity of equilibrium states, instability, and bifurcation). If this set of equations is really adequate to the physical one, the negative answer about long-term crop yield forecasts on large territories must be revised along with a series of other primary ideas about the cyclic character of natural phenomena.

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Crop Modeling: Nostalgia about Present or Reminiscence about Future

Ratmir A. Poluektov* and Alexandre G. Topaj

ABSTRACT

During the last two decades, computer simulation models have become powerful tools for investigating agricultural crop dynamics and solving practical problems. Many models have been developed in various countries, which permits exploration of the influence of weather conditions and agricultural strategies on the fate of a crop. However, some fundamental problems related to the description of agricultural plant growth and development remain unsolved. These primarily concern the totality of biological processes such as ontogenetic development and morphogenesis due partly to the lack of knowledge in plant physiology and the absence of realistic ideas about the origin of plant life. These circumstances have forced modelers to use quite sophisticated heuristic approaches rather than biologically sound descriptions. This paper represents the authors' vision of this situation.

THE APPEARANCE OF DYNAMIC MODELS in agroecology has led to a new understanding of the processes taking place in the soil–plant–atmosphere system and to formation of so-called *dynamic thinking*. The Russian school of crop simulation recognizes Monsi and Saeki (1953) as the originators of this new branch of science (this may deviate from the traditional Western point of view) (Sinclair and Seligman, 1996). Monsi and Saeki's approach was further developed by many authors in the former Soviet Union and, in particular, by a group of scientists at the Agrophysical Research Institute in St. Petersburg. Unfortunately, contacts between eastern European and Western scientists were rare for a long time, and agroecological simulation developed along separate courses.

Budagovsky and Ross (1966) proposed a theoretical approach to the quantitative description of crop photosynthetic activity. It was probably the first publication in Russian concerned with crop simulation. Later, Bik-

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hele et al. (1980) developed the model describing the processes of photosynthesis and transpiration under soil water deficit conditions. Sirotenko and Boyko (1985) created a complex set of differential equations for the simulation of energy and mass transfer in a crop. Our efforts (Poluektov et al., 1979; Poluektov, 1991; Poluektov and Vasilenko, 1993; Poluekotov and Topaj, 1996; Poluektov and Zakharova, 2000) were directed toward the development of theoretical as well as applied models. Various complex problems including such specific tasks as wheat (*Triticum aestivum* L.) wintering or account of soil moisture excess were addressed. As a result, a family of models was developed starting from simple constructions and finishing with very complex and detailed structures. Now we have a set of models adapted to several crops [winter and spring wheat, barley (*Hordeum vulgare* L.), maize (*Zea mays* L.), alfalfa (*Medicago sativa* L.), and others] grown in a number of different regions of Russia (Krasnodar, Saratov, Altaj, Leningrad, and Kaliningrad). It is possible to assert that these and other existing models together constitute the base of crop simulation knowledge, and it should seem that all of the principal problems in this field (especially since the appearance of modern powerful personal computers) are finally solved. But . . .

SCIENCE VERSUS UTILITY IN CROP MODELING

Computer crop modeling is now a power industry in itself with its own tasks, methods, and fields of application. So, it is useful to turn back and sum up the results from more than 40 yr of history. A careful observer may notice that there are two principal simulation philosophies corresponding to alternative approaches of algorithmic representation of the physical, chemical, and biological processes taking place in real agricultural ecosystems. The first approach is often called theoretical and the second one empirical, but in other works, one can find the terms mechanistic and functional or biophysical and heuristic. What is the main difference between the two methodologies in crop simulation?

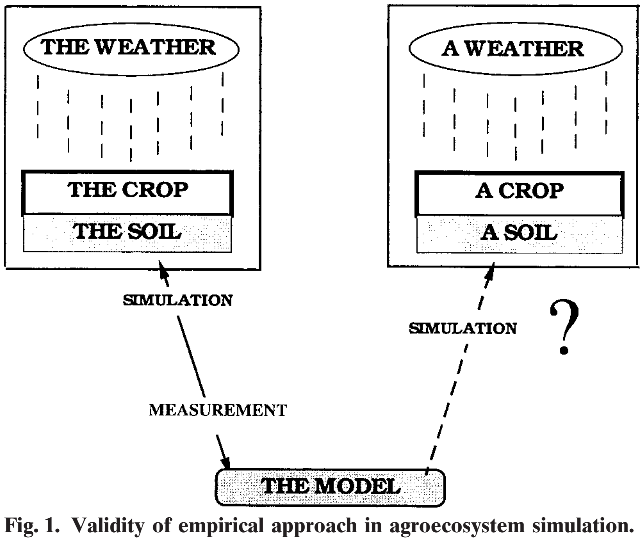

Fig. 1. Validity of empirical approach in agroecosystem simulation.

Models based on an empirical approach can be considered as a set of heuristic equations describing crop growth and development. Each of these equations is usually a static description of a relation between the rate of the considered process and environmental conditions. Input parameters for these equations must be identified using standard or specially planned field experiments. Insertion of these equations into simple dynamic algorithms yields an empirical model. It is easy to see the shortcomings of such a simple approach. Firstly, such models represent a return to the concept of regression analysis although on a new qualitative level. Complications arise if one increases the number of defining relations, resulting in additional difficulties for parameter identification.

An empirical model is not versatile, and in reality, can require too much time to identify model parameters for each specific set of crop, soil, and environmental conditions. In many cases, we can obtain excellent correspondence between measured and simulated data. However, one will never be certain that the developed model will be useful for the description of a different crop exposed to different soil and weather (Fig. 1). When these conditions change, the parameter values (this problem can be solved by reidentification) as well as the qualitative type of equations may be wrong.

The most impressive argument for the insufficiency of *curve fitting* methodology in crop modeling is the comparison of results from different models applied to the same data set. Such comparisons have taken place within the framework of various workshops or projects but almost always with the same consequence (Dieckkruger et al., 1995; Poluektov et al., 1999). Divergence in the results of production process simulation (for its various components, e.g., crop yield, soil water content, and phenology) is very high, sometimes reaching several hundred percent! So, which models can one trust?

Any attempt to extend the scope of an empirical model beyond the events or conditions for which it was developed and tested is not simulation but rather speculation. Therefore, the empirical approach to crop simulation cannot be used with confidence as a method of scientific investigation. A common example of its inapplicability is the currently popular modeling task connected with studies of the possible influence of global climate change on the ecological stability of agricultural systems. Probably the lone essential advantage of the empirical approach is that these models are available and can be successfully used for decision making in agriculture. As will be shown below, the theoretical models do not have this important property.

Theoretical approach means an *honest* description of crop and environmental dynamics and entails development of a mathematical model according to the physical, chemical, or biological principles underlying all of the processes included. A pure theoretical model consists of physically interpreted relations (unlike the logically interpreted ones in the empirical models). As a rule, they are the differential equations of mathematical physics, which follow from the consideration of energy and matter balance for selected spatial or functional compartments. Certainly, such a model could be used as a tool for scientific research. Its algorithmic content is not connected with the conditions of its adjustment and validation, and one can be sure that the laws of nature are more *universal* than human fantasies. There is only one difficulty (but it is global) in applying the theoretical approach to mathematical simulation of agroecosystems. The honest description of all of the processes included in the model, and especially their integration into the complex scheme with the same level of accuracy, is an extremely difficult problem. Some phenomena (mainly of a biological nature) have not yet been studied in sufficient detail. Theoretical models require developers to be skilled specialists in various branches of science. It makes the development of the mechanistic model so difficult that there still is no complex agroecosystem model that can truly be called theoretical. Probably the main success has been achieved in creating single units or submodels of separate processes in the soil–plant–atmosphere system. Their integration into a comprehensive model now seems to be a utopian dream.

Let us compare the two approaches, using as an example the photosynthetic units (blocks) of corresponding models. For the empirical case, the winter wheat model AGROSIM-WW [AGROecosystem SIMulation—winter wheat (WW)] has been chosen. It was developed by specialists at the Institute of Landscape Modeling (Muencheberg, Germany) and is a part of the AGROSIM model family (Wenkel and Mirschel, 1995). This model follows the typical pattern of empirical methodology. The main relation for calculating daily photosynthetic rate is given by the following multiplicative equation of partial stress functions:

$$F_D = F_M \times B \times f_1(\mathrm{QP}) \times f_2(\mathrm{TP}) \times f_3(\mathrm{BM}) \times f_4(\mathrm{WS}) \times f_5(\mathrm{WL}) \times f_6(\mathrm{NF}) \times f_7(\mathrm{CO_2}) \times f_8(\mathrm{DL})$$

where F_D is actual daily photosynthesis rate (kg ha^{-1} d^{-1}), F_M is biological maximum of assimilation per unit of green leaf biomass under optimal conditions, and B is total green biomass. The f functions are partial stress functions describing the relative decrease in primary assimilation under nonoptimal values of each of the following factors: QP, incoming solar irradiance; TP, phototemperature; BM, total biomass; WS, current soil water contents; WL, past soil water contents; NF, N content; CO_2, atmospheric CO_2 concentration; and DL, daylength. Each of these stress functions is a purely empirical dependency with the parameters identified from field tests. So, the main relation embodied in the equation can be easily interpreted but has no physical basis.

As an alternative, the model developed at the Agrophysical Research Institute for calculating daily photosynthesis rate (Poluektov, 1991) has been selected. It purports to meet the requirements of the theoretical approach. The algorithms used in the model consider the main physical and biochemical phenomena connected with photosynthesis and gas exchange in green leaves. The processes of CO_2 diffusion to the intercellular space from the atmosphere, chlorophyll excitement upon light absorption, and dynamics of biochemical reactions in the Calvin cycle are formulated as a set of differential equations. The model of leaf photosynthesis is extrapolated to the crop scale to produce a theoretical model of crop photosynthesis where each macroparameter has a concrete physical meaning.

Comparison of model run calculations using the same input data clearly demonstrates the advantages and disadvantages of each approach. Note that there were no specific calibrations of either model before comparison. There are some conditions where the theoretical model produces results that are quantitatively and qualitatively similar to the empirical model (Fig. 2). It is more interesting, however, to consider the circumstances where they vary. Some of these cases suggest an advantage to the empirical approach (Fig. 3). For instance, results of the AGROSIM model show the well-known unimodal dependency of photosynthesis rate on phototemperature while the theoretical model does not take this feature into account (Fig. 3A). We can review our theoretical model to correct this mistake, but we can never be certain to avoid another absurd result. However, the theoretical model has an important advantage—it can give new, unexpected, and scientifically valuable results as shown in Fig. 4 where the joint influence of two factors on photosynthesis rate has been investigated: atmospheric CO_2 concentration and water stress. For the empirical model, one can see that the C curves of photosynthesis are qualitatively similar under various levels of water availability (Fig. 4B). The results are different with the theoretical model. Under unstressed conditions, CO_2 concentration in the atmosphere is nearly at the saturation point and further increase has little effect on the photosynthesis rate. However, under conditions of strong drought, the dependency of photosynthesis on CO_2 concentration is practically linear. This result is correct; it has been confirmed by experimental results from greenhouse experiments. This mechanism was not explicitly included in the model during its development, so we have used the model as a tool of scientific research and gained new knowledge as a result.

During the past 30 yr, and especially for the past few years, we have had to maneuver between scientific and utilitarian thinking in crop simulation. Indeed, progress in the development of modern hardware has removed many of the previous restrictions concerning computer resources. This provides a basis for improving empirical models and closing the gap between empirical and theoretical approaches. Some efforts have been made at the Agrophysical Research Institute to fulfill this promise. As an example, two proposed methods for describing physiological processes in the plant canopy are presented below.

The first is a new method for simulating actual values of plant transpiration and soil evaporation (Poluektov et al., 1997). The well-known Penman–Monteith approach was used as a basis for our method (Penman, 1948; Monteith, 1981). However, our approach differs in two respects. Only the radiation absorbed by phytoelements is included in the heat balance equation, and the depen-

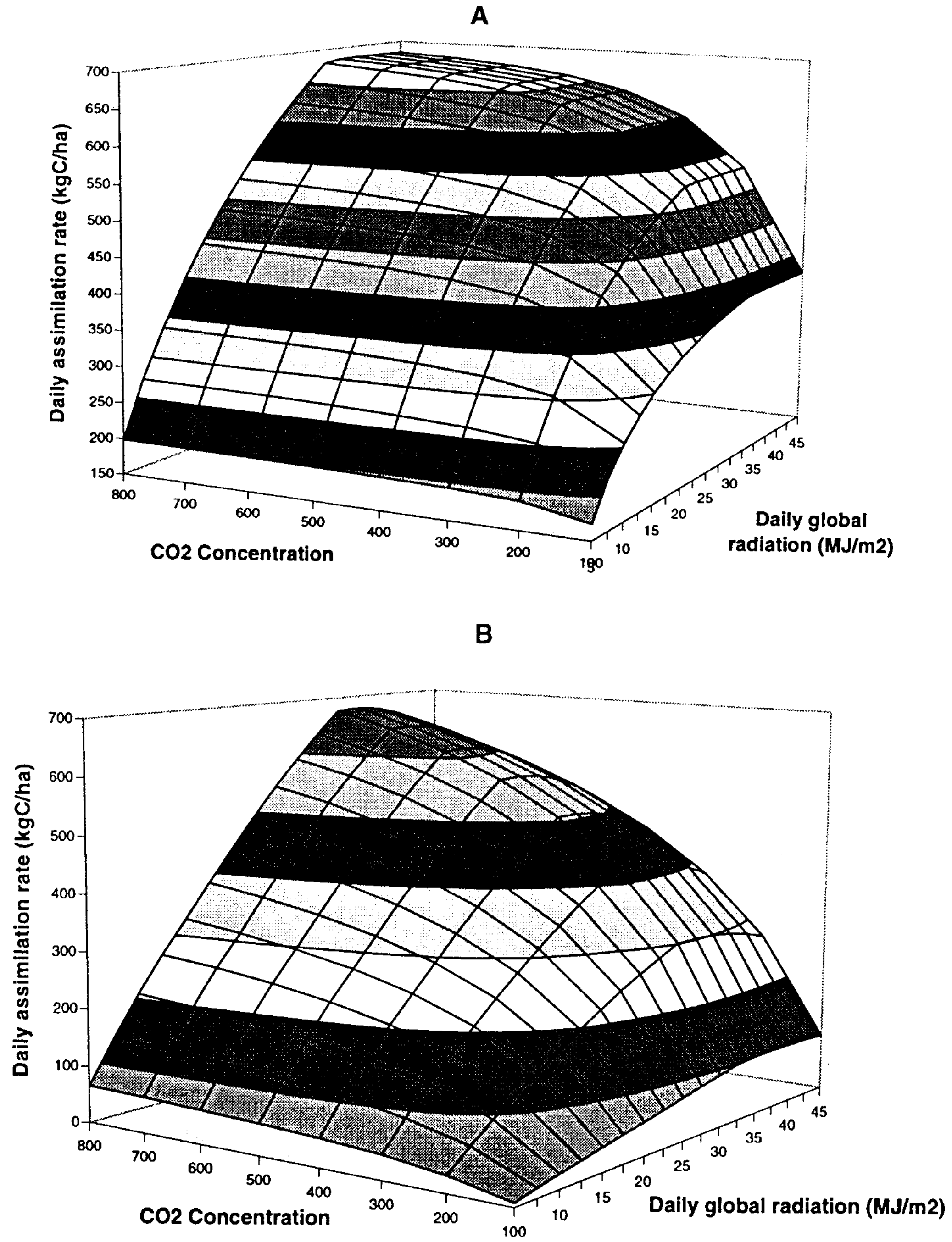

Fig. 2. Function of daily photosynthesis rate vs. global radiation and CO_2 concentration for (*A*) a theoretical model and (*B*) an empirical model.

dence of stomatal resistance on leaf water potential is used to calculate the actual value of plant transpiration as influenced by weather conditions and leaf water potential. The method accounts for the physical processes in the soil and atmosphere as well as for the physiological characteristics of water transport in plants. It takes into account the water deficit and its impact on crop dynamics. In addition, a new technique has been proposed for description of the opposite situation—the influence of water excess (and consequently, soil O_2 stress). The main idea was to include a unit in the model to describe the exhaustion of internal plant energy resources under saturated conditions, i.e., in the case when soil water content exceeds field capacity. A similar approach has been proposed for the calculation of evaporation from the upper soil layers.

The second method is a new algorithm for the simulation of dry matter distribution between shoot and roots. It can be called an *adaptive distribution key*. A fixed distribution key is usually used in models of annual crops (Penning de Vries et al., 1989). It does not allow description of plant reactions to environmental conditions such as soil water and N regimes. However, some processes are affected by the C and N content of the plant organs, for example, CO_2 assimilation by green parts of the plant and N uptake by roots. Consequently,

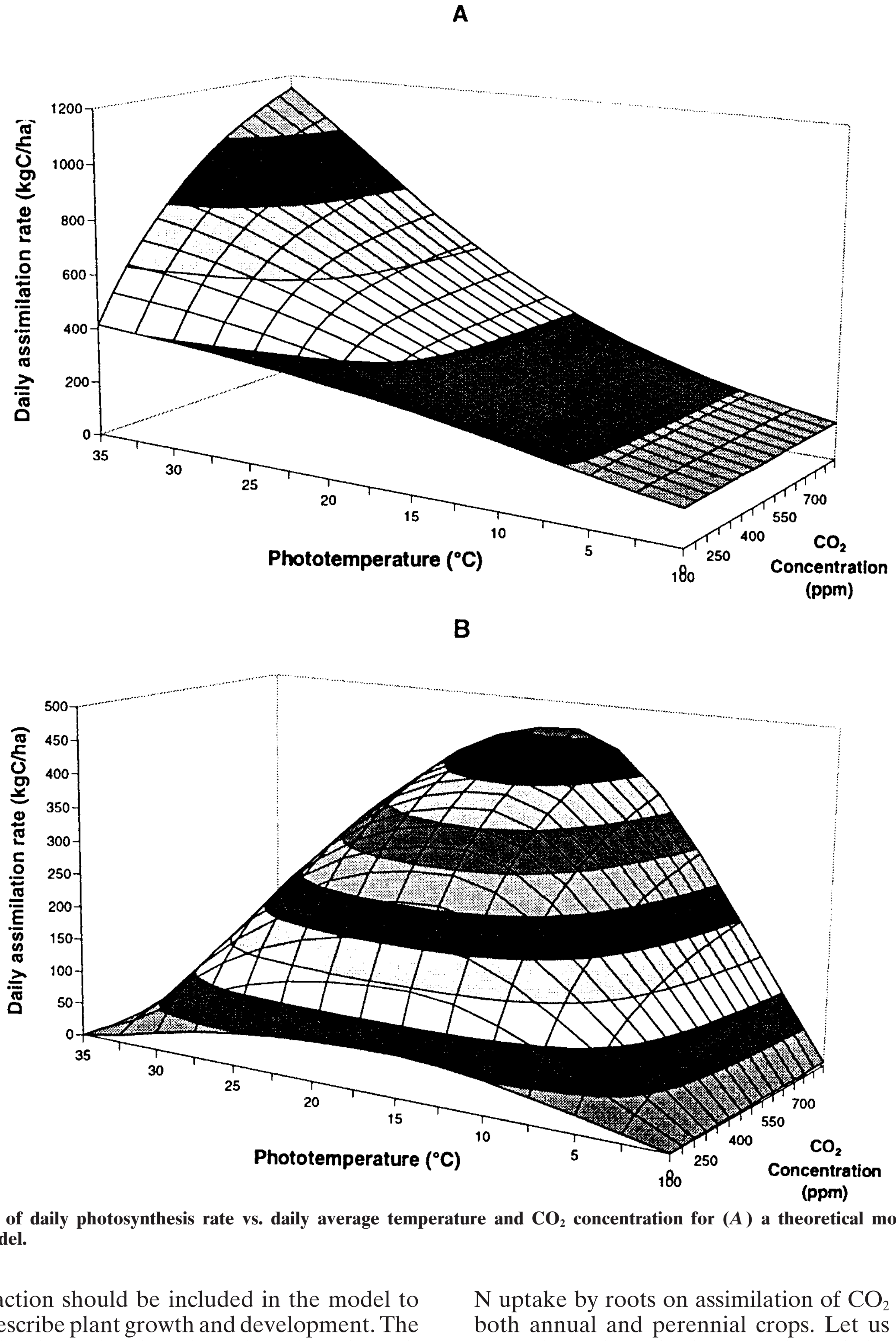

Fig. 3. **Function of daily photosynthesis rate vs. daily average temperature and CO_2 concentration for (*A*) a theoretical model and (*B*) an empirical model.**

C × N interaction should be included in the model to adequately describe plant growth and development. The method that has been developed was based on the estimation of a fraction of daily assimilates, which are either translocated into roots or remain in the leaf according to N demand and availability (Poluektov and Zakharova, 2000).

Our goal was to describe an alternative mechanism for dry matter partitioning that reflects adaptive crop reactions to ambient conditions, especially the effect of N uptake by roots on assimilation of CO_2 by leaves for both annual and perennial crops. Let us consider the example of alfalfa in the second or third year of vegetation. In this case, there is a large amount of roots and a small amount of aboveground dry matter during vegetation renewal in spring or after a recurrent cut. The high N availability leads to the primary growth of green plant organs so that accumulated carbohydrates limit plant growth. Root dry matter decreases due to respiration. When shoot dry matter reaches the compensation

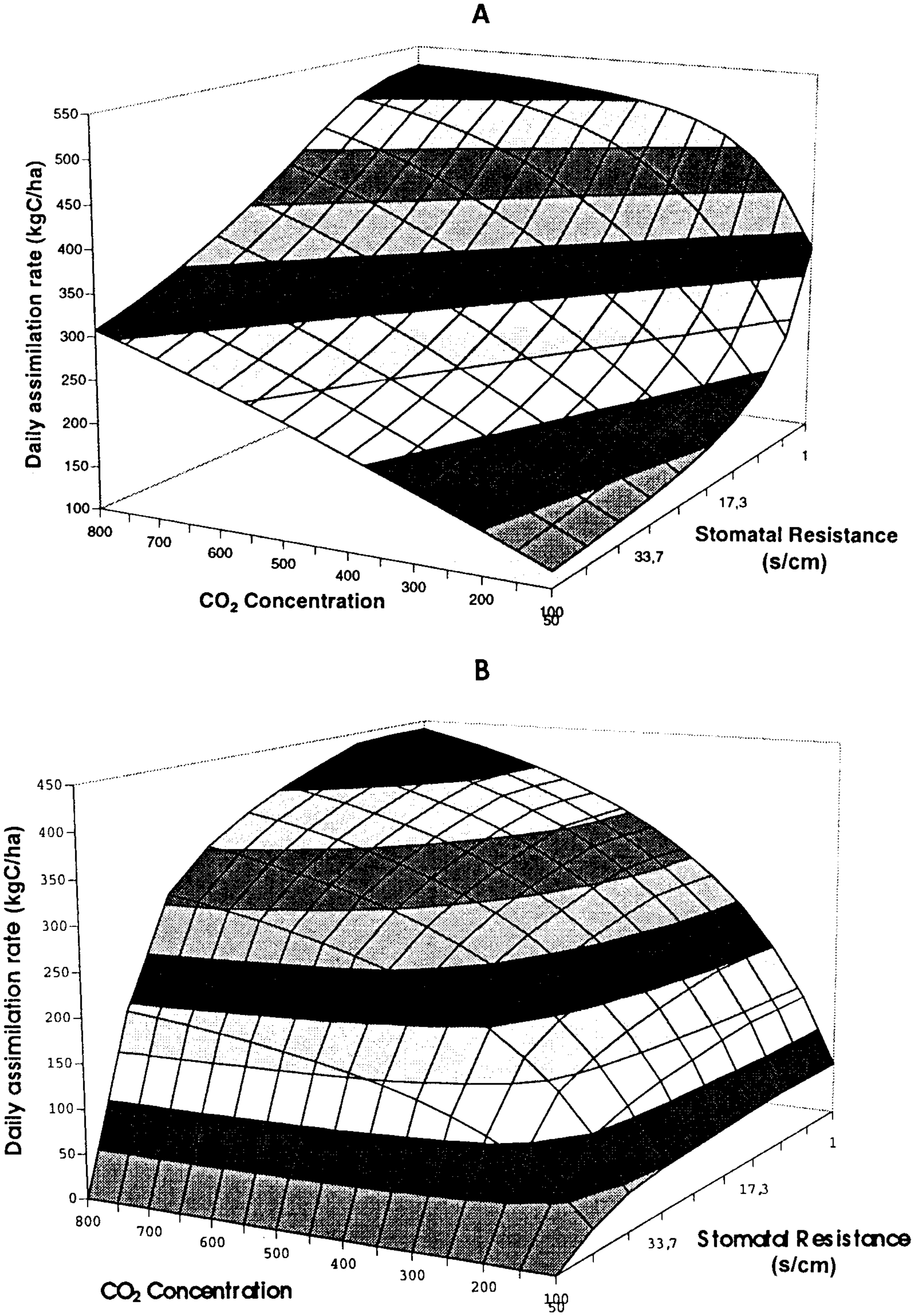

Fig. 4. Function of daily photosynthesis rate vs. water stress index (stomatal resistance) and CO_2 concentration for (*A*) a theoretical model and (*B*) an empirical model.

point and excess carbohydrates are produced, a fraction is translocated into roots so that dry matter rises again. The whole picture is clarified in Fig. 5. It demonstrates the *sawtooth* time course of the aboveground biomass and the oscillatory nature of root biomass dynamics. Because the daily amount of assimilates produced by photosynthetic organs depends on the current weather conditions, this distribution key reflects adaptive plant reaction to environmental conditions, thus the name, adaptive distribution key.

DISCUSSION AND CONCLUSIONS

Summarizing our vision, we can state that, in general, empirical models produce results that are usually reasonable, not always correct, and never scientifically val-

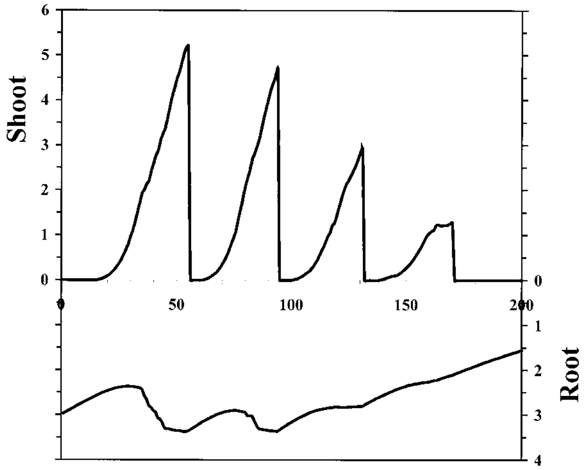

Fig. 5. Simulated dynamics of shoot and root dry matter of alfalfa during the vegetation period.

uable. Conversely, theoretical models produce results that are not always reasonable, rarely correct, but sometimes unique. Thereby, the modern situation in crop modeling leads to the formulation of two main questions: Is it now possible to use empirically developed models in scientific research to obtain new knowledge? Is it now possible to develop complex theoretical models to describe a crop with an acceptable level of adequacy? It seems that the answers to both questions are negative. This rather pessimistic conclusion requires modelers to delineate possible ways to further develop crop simulation. Two different opinions are possible.

The first one is that it is necessary to clearly share the sphere of application of our efforts. Empirical models must contain a minimum of scientific complexity. They must be as simple as possible and should provide very accurate results for a broad class of environments. On the other hand, their area of application must be limited to the solution of utilitarian problems (e.g., operative crop control and management during vegetation period or yield forecast). The primary tasks facing empirical modelers are probably the changing of model interfaces and the coupling of computer crop models with the modern tools and products of information technologies (such as geographical information systems, object-oriented modeling systems, remote database servers, and others). One can see many practical applications in this direction.

The second opinion is that theoretical (scientific) simulation must focus on the honest and detailed description of partial processes, realizing that the development of the complex, fully theoretical model is an endless and hopeless cause.

The alternative point of view is more optimistic. Some positive modeling examples demonstrate the idea that by taking into consideration more physical or biological descriptions of various processes, it is possible to extend the scope of application of both theoretical and empirical models. Certainly, the number of holes in the existing models is still too high to dream about the appearance of a good complex model in the near future. But we must note that success comes to the patient researcher only. It is difficult to say which of these opinions about future development is more correct. Most likely, the truth is somewhere in the middle.

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