International Conference
20th EURO Mini Conference
"Continuous Optimization and Knowledge-Based Technologies"
(EurOPT-2008)
May 20–23, 2008, Neringa, LITHUANIA

ISBN 978-9955-28-283-9
L. Sakalauskas, G.W. Weber and
E. K. Zavadskas (Eds.): EUROPT-2008
Selected papers. Vilnius, 2008, pp. 87–92

SIMULATION OF PLANT PHENOLOGY IN COMPLEX AGROECOSYSTEM MODELS AS AN OPTIMAL CONTROL PROBLEM

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Abstract: Basic requirement to use the computer crop model for scientific analysis is a theoretical character of formalization of ecosystem properties and behavior. Hence, one of the main challenges in physiologically-oriented dynamic models of plant growth and development remains the proper mathematical description of biotic regulation processes in plant ontogenesis. The perspective approach to reflect the visible patterns of plant behavior in non-stationary environment is the idea about its optimality as a result of evolutionary natural selection's pressure. So, the principal aspect of the use of optimal control theory in plant modeling unlike technical applications is not to optimize something but to express existing features in plant development, i.e. to deduce them from rather simple assumptions. The contribution focus is to present the new approach for simulation the plant phenological development in the framework of the comprehensive agroecosystem model. The task is formulated as a traditional problem of optimal control containing two dynamical variables corresponding with vegetative and generative parts of the simulated plant. The objective in optimization problem is the power (biomass) of generative organs at the end of vegetation period. Case study of presented model demonstrates the non-trivial behavior of the optimal solution. Depending on model parameters it can be the expected as "bang-bang" strategy (strongly separated periods of purely vegetative and purely generative growth) as well as more complex strategy containing the period of singular control (the growth of vegetative and generative organs take place simultaneously). The results can be interpreted as an original explanation of really observed principal patterns of phenological development for annual as well as perennial plants.

Keywords: optimality principle, plant phenology, growth curve, singular control, vegetative-generative switch, dry matter distribution.

1. Introduction

During the last three decades computer simulation models turn into the powerful tool for investigation and scientific analysis of agricultural crop dynamics as well as for the solving of practical problems. There are a lot of models developed in various countries and organizations which permits to reflect the influence of weather conditions and agricultural strategies on a crop fate. These models differ by many criteria, but one can notice that there are only two principal ways of simulation philosophy (Poluektov, Topaj, 2001). They both correspond to the alternative approaches to algorithmic realization of a set of physical, chemical and biological processes taking place in the real agricultural ecosystem. The first approach can be called theoretical (mechanistic, biophysical etc.) and the second one empirical (functional, heuristic etc.)

The models created on the base of empirical approach can be considered as a set of heuristic equations, describing crop growth and development in terms of static relations between the rate of the considered process and the current environment conditions. The parameters of equations must be identified using standard or special field experiments. The approach is the typical pattern of «curve fitting». The nature is considered as a «black box», described by means of «input-output» ratios, each of them can be rather easily understood in intuitive level, but has no physical essence.

An empirical model can not be called versatile one. Indeed, we spent much time to identify the quantitative values of model parameters for the concrete crop, definite soil and given environmental conditions. We can obtain an excellent coincidence between empirical and simulation data. However, any attempt to extent the scope of application of empirical model to the events or conditions, which could not be created or tested experimentally is not simulation but rather speculation. So, the empirical approach to the simulation can not be used with confidence as a method of real scientific investigation.

Theoretical approach means «honest» description of crop and environmental dynamics and requires implementation the mathematical model according to physical, chemical or biological essence of all the processes. Pure theoretical model consists of **physically** interpreted relations (unlike of **logically** interpreted ones in the empirical models). As a rule, they are the differential equations of mathematical physics, which follow from consideration of energy and matter balance for selected spatial or functional compartment. Certainly, this model could be used as a tool of scientific research. Its algorithmic content is not connected with the conditions of its adjustment and validation. Really, one can be sure, that the laws of nature are more «universal» than human fantasies.

Any existing agroecosystem model is, in practice, the mixture of empirical and theoretical approaches. At that, the algorithmic modules describing the abiotic processes in soil and athmosphere are, usually, more «theoretical» than the biological modules. Description of corresponding processes, as a rule, is based on the balanced equations following mass or energy conservation lows. We have not yet such universal qualitative lows in biology. Hence, theoretical method for description of the plant physiology process is inevitably more subjective. It is especially so for the **regulation** processes (organogenesis, phenology, dry matter distribution) in contrast to **metabolism** processes (photosynthesis, respiration, transpiration). Roughly speaking, the plant growth (qualitative dynamics of organ biomass) can be in theory adequately described by more or less well-grounded relations but not the plant development (i.e. quantitative transformations in ontogenesis).

As it mentioned above, the only theoretical model can be useful for really scientific analysis. So, the determination of theoretical base for mathematical formalization of regulation processes remains the main challenges for the specialists in mathematical simulation in plant eco-physiology. The dream is to find a general principle, any common paradigm solving this problem.

2. Optimality principle as a common paradigm of the modeling regulation processes in plants

The idea to explain the visible patterns of plant form and behavior by means of optimality consideration is not new or original. Optimization is about making something, generally a complex system of interacting elements as fit as possible. In the framework of biology we say «fit» and understand «survival». Indeed, Darwin's theory of evolution by natural selection admits that natural selection leads to an optimization process, meaning the organisms better fitted to their environment will have a selective advantage. It is well-known the Spencer's phrase «Survival of the fittest». This sentence can be inverted to the form «Survived is optimal». It means, we don't try to shed light on the way in which natural (existing) organisms relate to their physical and biotic circumstances and it is that particular phenotypes correlate with particular environments. That is to engage in what has been termed «reverse engineering»: identification of the attributes and the behavior lows of an organism that contribute to its being fit. The good analogy is the comparison of Lagrange's and Newton's formalism in classical mechanics. According to Newton, the behavior of dynamic system can be described in terms of causes and consequences (forces and accelerations). The alternative Lagrange's approach (analytical mechanics) operates the terms of objectives and abilities (action and constraints). To describe the mechanical system in classical mechanics is to define the vector of the forces for the every mass point and to solve the obtained system of differential equations. To do it in analytical mechanics is to solve the single variation problem (search of the optimum of scalar functional in the set of constraints). The main idea of application of optimality principle in plant models is to use something like Lagrange's formalism in biological applications. The principal challenge here is the choice of the goal of optimization. For the considered problem (simulation of regulation processes in plants) the cornerstone principles of the approach can be formulated as following:

- Individual plant is considered as a complex dynamic open system (upcoming and cyclically self – reproducing mechanism) with the definite objective of its existence
- The objective is formulated in terms of reproducing of the most powerful (quantitatively and qualitatively) descendants
- The lows of metabolism (producing and transport of structural matter inside plant) are known and invariable
- The investigated regulation process is considered as the program controlling the metabolism. It can be expressed as the set of control directives depending on external conditions and/or feedbacks depending on internal variables
- The purpose of the control is achievement the optimal value of the objective variable, i.e. the control program can be found as a solution of optimization problem.

The principles seem to be abstract and banal. But it can be shown, that their application can demonstrates the non-trivial results and be useful in solving many problems concerning mathematical descriptions of different regulation processes in plants. One of the examples is presented below.

3. The model of vegetative-generative plant growth

Traditional methodic to describe plant phenology in complex agroecosystem model is the approach based on so called «biological time» - artificial dynamic variable integrally computed from the weather characteristics and indicated the quantitative index of plant development – from infancy to maturity. So, the trigger for the every next phonological stage is the moment, when «biological time» value attains corresponding threshold. The empirical, heuristic nature of the approach is obvious.

Alternative way is to apply the above mentioned common paradigm – optimality principle. A major development transition in higher plants is the switch from vegetative to reproductive growth. To maximize reproductive success, it is essential that the timing and the level of this transition is correct. Moreover, not only correct, but optimal. Let's try to express the sentences in mathematical form.

We've chosen a very simple model of plant structure. The biomass of an individual plant is divided into two parts: vegetative (V) and generative (G). At the start of the growth $V = V_0$ (i.e. seedling size after germination) and $G = 0$. The only essential metabolism equation is the rate of assimilation producing which depends on the power of vegetative organs and non-stationary environmental conditions (temperature, solar radiation etc.). The primary assimilates (growth resources) are allocated between the generative and vegetative parts at a given time. The allocation schedule is optimized to maximize the final size of the reproductive compartment, $R(T)$, where T represents the end of the analysis period. The resource allocation to the vegetative components at time t is denoted by $u(t)$ which is the control variable of the problem. The constraints for the control are the natural limitations $0 \le u(t) \le 1$. Given these assumptions, the dynamics of biomass allocation to vegetative and reproductive parts of a plant are expressed by the following equation system:

$$\begin{cases} \dfrac{dV}{dt} = u \cdot A(V,t) - \lambda \cdot V \\ \dfrac{dG}{dt} = (1-u) \cdot A(V,t) \end{cases}, \tag{1}$$

where $A(V,t)$ is the rate of assimilation, λ – rate of vegetative biomass decay due to respiration. The individual plants in question uses an $u(t)$ that maximizes the final size of the reproductive part $G(T)$, i.e. the formulation of optimization functional is:

$$J = G(T) = \int_0^T \frac{dG}{dt} \cdot dt \to \max . \tag{2}$$

4. Model analysis

Such a problem can be solved by Pontryagin's maximization principle. Based on (1), the Hamiltonian formulation is

$$\begin{gathered} H = u \cdot A(V,t) \cdot P_V - \lambda \cdot V \cdot P_V + (1-u) \cdot A(V,t) \cdot P_G = \\ u \cdot A(V,t) \cdot (P_V - P_G) + A(V,t) \cdot P_G - \lambda \cdot V \cdot P_V , \end{gathered} \tag{3}$$

where P_V, P_G – are co-state variables for V and G correspondingly, expressed by dynamic equations:

$$\begin{gathered} \frac{dP_V}{dt} = -u \cdot \frac{dA(V,t)}{dV} \cdot P_V + \lambda \cdot P_V - (1-u) \cdot \frac{dA(V,t)}{dV} \cdot P_G \\ \frac{dP_G}{dt} = 0, \end{gathered} \tag{4}$$

with boundary conditions following by their nature (response function of the objective on dynamic variables):

$$P_V\big|_{t=T} = 0; \qquad P_G\big|_{t=T} = 1 . \tag{5}$$

Taking into account assimilation rate $A(V, t)$ is positive, the low of optimal control according to (3) is expressed by:

$$u_{opt}=\begin{cases}1, & P_V > P_G\\ 0, & P_V < P_G\end{cases}, \tag{6}$$

i.e. optimal resource allocation strategy for the problem is almost always the «bang-bang» control. The only exception is the case $P_V = P_G$, where the control following by Pontryagin's method remains uncertain. The complete analytical or numeric case study of optimal solution requires additional assumptions about the shape of assimilation function *A(V, t)*. Let's consider several simple examples.

4.1. Linear growth in constant environment

The case corresponds $A(V,t) \equiv a \cdot V$, where constant assimilation rate a is greater than λ (otherwise the growth is impossible). For the assumptions the problem (1–5) can be solved analytically and we receive

$$u_{opt}=\begin{cases}1, & t < T^*\\ 0, & t \ge T^*\end{cases}; \quad T^* = T - \frac{1}{\lambda}\cdot \ln\frac{a}{a-\lambda}, \tag{7}$$

so, the optimal strategy is the pure «bung-bung» control and the greater net-assimilation rate the after must occurs the time of the switch from pure vegetative to pure generative growth.

4.2. Non-linear growth in constant environment

It is known, linear dependency of assimilation rate on biomass is not proper model of plant production process. In reality photosynthetic ability increases more slowly than the size of the vegetative component because a large vegetative part may be accompanied by increased maintenance cost or low light intensity due to self-shading. Moreover, corresponding ratio must have saturation point where increase of biomass does not increase assimilation. Let's choice the appropriate relation in form:

$$A(V,t)=\frac{a\cdot V}{1+V/V_M}, \tag{8}$$

that is so-called Michaelis-Menten equation wide-distributed in biophysics and biochemistry. Being coupled with the first equation in system (1) this formulation gives a sigmoid curve as a low of vegetative biomass dynamics during pure vegetative stage of development. The inflection in this case occurs when biomass value is equal to V^*, where

$$V^* = V_M \cdot \left(\sqrt{\frac{a}{\lambda}} - 1\right). \tag{9}$$

Analytical solution of optimal control problem is, in case, practically impossible, so we used the numerical calculations to investigate the task. We have the system of two differential equations with boundary conditions at the beginning and at the end of integration interval, i.e. Cauchy problem. The proper solution method was to apply the «zeroing in» method in «reverse» time. The results obtained are not trivial. It turned out, that the solution, expressed by (6), i.e. «bang-bang» control exists only for definite area of the parameter region (V_0,T) $(V_0,T)\ |0 < V_0 < V_0^{cr}(T)$. For the values $V_0 > V_0^{cr}(T)$ the Cauchy problem expressed by (1), (4–6), (8) has no solution. It means that the pure Pontryagin's formalization may be insufficient here to find the correct solution.

We used the alternative approach to find the optimal control for the problem in any area of parameters. It is based on Bellman's dynamic programming method. The main idea is to write the little variation of Bellman's attainability function in terms of the second infinitesimal order. It allows obtaining the following low of optimal control (the corresponding calculations and the evidence of the below mentioned conclusions are omitted by the reason of their complexity)

- There are three principal cases forming the different patterns of optimal strategy of resources allocation in the formulated problem and defined by the set of parameter values.
- If initial value of vegetative biomass V_0 is rather big and the expected growth period T is rather small than the optimal control consists of generative growth only. It has no biological meaning.

- For the definite ratio between V_0 and T optimal strategy is the «bang-bang» control. The plant allocates all of its resources to vegetative growth early in the season and reproductive growth later in the season. At that, during first stage the vegetative biomass increases to a certain value, which can be always less than inflection V^* (curve 2 in Fig. 1).

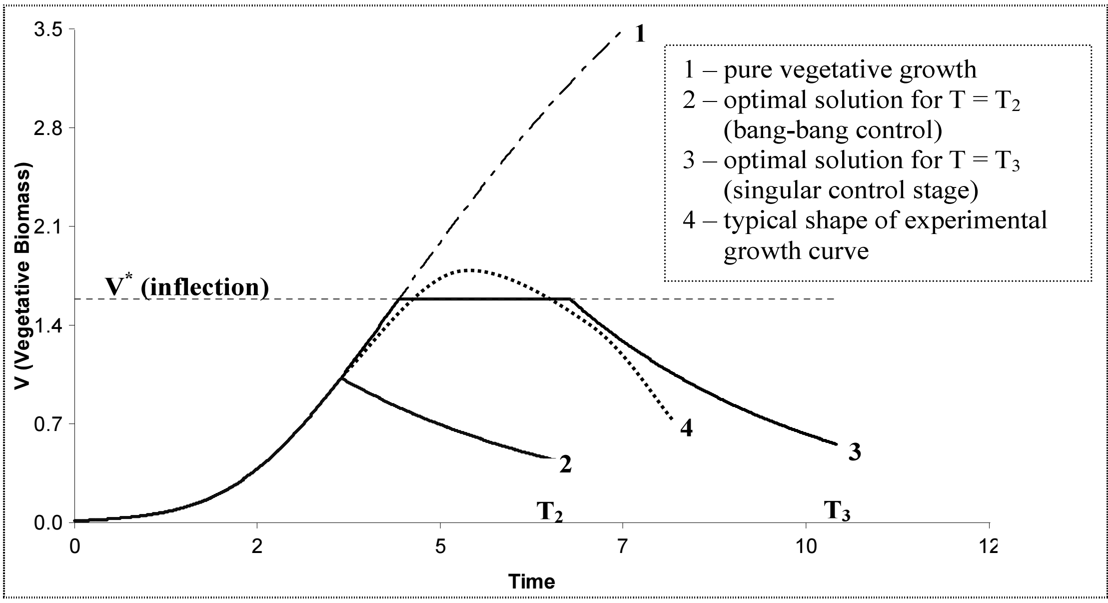

Fig. 1. Vegetative growth curves for different optimal allocation strategies

- For rather long vegetation period T, optimal strategy consists of three stages. Firstly, plant invests exclusively in vegetative component, whereas it contributes to both vegetative and reproductive parts in the middle of the season and only to the reproductive part toward the end of the season. The first stage is continued until the value of vegetative biomass increases to V^*, that is the trigger of second stage begin. The control strategy on the second stage is to keep the value of vegetative biomass at the constant value equal to V^*, so the inflection can also be called the point of optimal retention. It is easy to see, that the growth curve for the case (curve 3 in Fig. 1) has a smoother shape than in «bang-bang» control assumptions. It is not the only possible explanation for the fact of the smoothness of plant growth curves observed experimentally (curve 4 in Fig. 1). But it is one of these.

Let's note the following. It is a wide-distributed mistake, that «bang-bang» control is the only possible solution of the optimal control problem for the cases, where both objective functional and dynamical variables are linear function of control variable. The task considered is an example refutes this statement. One can see, that the non-trivial, border form of the solution (so called «singular control») is not the only mathematical abstraction, but can occur in real tasks even in biology.

4.3. Non-linear growth in non-stationary environment (perennial plants)

Finally, consider the following expression for assimilation rate

$$A(V,t) = \frac{a \cdot \left(1 - b \cdot \cos(\omega \cdot t)\right) \cdot V}{1 + V/V_M} \quad . \tag{10}$$

The last formula is an extension of (8) for the case of non-stationary external conditions. We proposed that the successfulness of environmental characteristics (temperature, radiation) for the assimilation varies according to harmonic curve. It is logic to interpret this additional dynamics as an annual oscillation, i.e. to consider the integration interval T as a long-term life period for perennial plants. The corresponding optimal control problem has been solved numerically and demonstrated the following results:

- If the environmental conditions vary significantly (amplitude b has rather big value) the pattern of resources allocation is such. Several initial years (infancy) the growth of the plant is pure vegetative. It corresponds to juvenile stage of ontogenesis. Later the stage of pure vegetative growth as well as the stage of generative growth occurs every year. And the bearing period concurs with decreasing branch of the annual dynamics of environmental successfulness («autumn» for northern hemisphere). Moreover, the total outcome of expropriated generative biomass becomes more than a plant becomes older. As is easy to see, such a development pattern coincides in full with widely known behavior of so-called polycarpic plants (fruit trees, for example)

- At the other hand, when amplitude *b* is not so significant («winter» does not so differ from «summer») development pattern is other. In this case perennial plant behaves like annual one. Namely, the optimal resource allocation is a «bang-bang» control with the single switch between pure vegetative growth during infancy (it can last many years) and pure generative growth at maturity. It is so called monocarpic perennial plants. It is interesting, that all known ones in wild nature (agave, some bamboo varieties) have their natural habitat in tropical latitudes, i.e. where the difference in environmental conditions during year is really minimal.

5. Conclusion

Use optimality principle in crop modeling is often subjected to criticism. The traditional argument against «teleonomic» models is that they do not satisfy the cornerstone paradigm of scientific research – the convention about the objectivity of the nature (Thornley, 1998). Other wide-distributed objection is that the «mathematical games» with optimality can explain everything, so the hypothesis cannot be falsified and, consequently, according to basic Popper's criterion, is unscientific (Mäkelä *et. Al.*, 2002). The arguments are serious. But there is another informal criterion in order to estimate the value of scientific theory. It is the ability to explain the complex phenomena observed in reality by means of rather simple and transparent initial assumptions. Optimality approach in plant physiology satisfies this criterion. And it refers not only to the simulation of crop phenology. It can be shown, that optimality can be also successfully applied for modeling organogenesis (Topaj, Poluektov, 2005), stomatal regulation (Cowan, 1977) etc. Moreover, it is now the only approach for description of regulation processes in plants in the framework of complex crop model having at least elementary scientific ground.

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