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## CROP MODELS AS RESEARCH AND INTERPRETATIVE TOOLS

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### Abstract

Mechanistic (eco-physiological), or process-oriented, approach to simulation modeling of the production process of plants assumes considering the essences of processes and cause-effect relationships in the agroecosystem with a description of their dynamics based on physically interpreted dependencies (as opposed to logically interpreted dependencies at the empirical approach) (A. Di Paola et al., 2016; R.A. Poluektov, 2010). The analysis of the possible use of dynamic simulation models of agro-ecosystems in the mechanistic nature of applied and theoretical research of agricultural biology is presented. The current practice of the development and usage of these models shows their highest suitability for research purposes in comparison to the potential usefulness and relevance to the practical problems of agronomy. Specific examples of model applications demonstrate the possibility of computer-based model experiments to get nontrivial results, which are not directly incorporated into the logic of the model algorithms (V. Badenko et al., 2014; S. Medvedev et al., 2015). The role of simulation model as a tool of obtaining new knowledge and interpretation of the empirically observed phenomena has been showed. To demonstrate the potentials of simulation models for agricultural biology, some results of authors' studies have been reviewed, including analyze of the appearance of a non-monotonic response function of crop yield on the doses of nitrogen fertilizer, the results of computer experiments on interpretation of the effect of the time delay during management of nitrogen feeding «on the leaf», and the joint impact of combined water and nitrogen stresses. Based on analysis of recent publications, conclusions of perspectives of models application to accelerate the plant breeding process were justified. It is concluded, i) further «biologization» of existing models is a prerequisite for a successful development of the dynamic crop growth modeling, and ii) it is necessary to increase the level of scientific validity of model approaches, which are used to describe the biotic processes in the soil—plant—atmosphere system.

Keywords: agro-ecosystems simulation model, crop production process, mechanistic approach, ideotype, plant breeding, breeding, G×E×M-oriented models

Imitation modeling of the plant production process is an independent scientific field with its own methodology, history [1, 2] and qualitatively different approaches to creation and use of computer models. In foreign literature, these approaches are traditionally designated as mechanistic, or process-oriented and empirical ones [3]. The empirical (functional) approach is characterized by broad application of heuristic description of key processes using regression ratios, allometry equations, multiple stress functions, etc. Such formal description at the logical level may perfectly reflect the properties of a real system in the "entry-exit" terms within a relatively narrow class and a limited range of affecting factors but is almost not associated with the essence of physical, chemical and biological effects in the soil—plant—atmosphere system [4]. On the contrary, the mechanistic (eco-physiological) approach implies considering the essence of processes and cause-to-effect relationships in the agroecosystem with description

of their dynamics based on the physically interpreted dependencies (in contrast to the logically interpreted dependencies at the empirical approach). The mathematical apparatus of the theoretical models are a system of differential or difference equations, as a rule, describing the balance of matter and energy for each of the considered spatial and functional compartments. The number of factors and processes, which should be taken into the account for providing a complex, stable and non-contradictory model of yield formation in the sowing within the fully mechanistic approach, severely hinders achievement of such an aim. Therefore, currently basic models of production process [5], which are a synthesis of process-oriented and empirical descriptions, pretend to be scientifically justified.

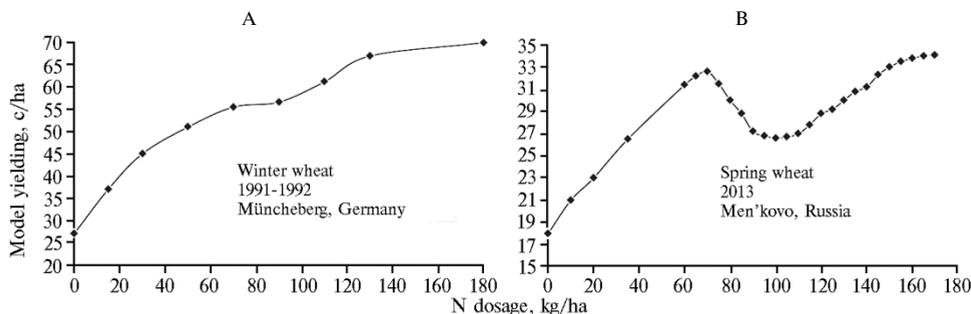
When the theory and methodology of imitation modeling appeared in agroecology, an issue was raised about the applicability of computer models. Five aims were designated [6], in accordance with which a hypothetical ideal model of the plant production process can be a communication means for specialists, a means of cognition, learning and purposed planning of experiments and an instrument of making decisions to control complex systems. The first two roles are rather related to purely theoretical studies, and the latter three ones are closer to practical agronomy. For a long time, there was an unspoken certainty among specialists that good process-oriented model can be successfully used for achievement of all five aims. However, at the end of the 20th century, doubts were expressed [7], and in the last 20 years, a directly opposite impression has formed. Many publications repeatedly state that there is no universal mathematical model to be equally applied both in theoretical studies and in practical calculations and predictions for wide spatial and time scale, and it is impossible to provide such a model in principle. Therefore, a correct strategy is not to constantly improve some single model platform in order to obtain a universal calculation tool but to create specifically narrowly oriented solutions for each specific problem (ad hoc modeling) [8].

In the world practice, the usefulness of most provided complex basic models for the agricultural production tasks (a support system for technological solutions, operative prediction of yield, mass calculations of potential productivity) appeared to be quite low [9-11]. Planning and controlling authorities use proven simple empirical models (agrometeorological predictions) of the expected yield of the main crops, and the involvement of satellite images and other remote probing data apparently completely resolves an issue of using such a complex instrument as process-oriented imitation models. In precise agriculture, their use also did not develop quite well: the number and variety of factors of inter-field heterogeneity significantly overcomes the functional possibilities of even the most advanced modern models. Moreover, the real variability degree of the determining parameters formally tuned in the most models (water stress, nitrogen nutrition, etc.) is often below the sensitivity threshold of the model algorithms; therefore, statistical models are most often used here [11]. Thus, for agronomical practice most process-oriented models appeared to be no better than their empiric analogues.

A popular application for imitation models could be theoretical science, specifically theoretical agricultural biology. Until recently, most biologists (if bioinformatics and molecular level genome studies are not referred to) were skeptical of computer experiments as a means of cognition and interpretation of observed events. They doubt a possibility of obtaining principally new knowledge from a model, which has been charged only with known facts and regularities. However, for process-oriented models it is only partly correct. At investigation of models that are indeed science intensive, new phenomena may be found or

original explanation for events observed in nature can be found, and such models themselves may serve as an intrinsically valuable scientific instrument and effective replacement of a field or lab experiment. We would confirm this statement below by examples of some mini-discoveries and explanatory hypotheses obtained by us in computer experiments with the models we have developed. First of all, emergent (i.e. not clearly charged to a model) unexpected effects exhibited as a result of and not clearly following from sufficiently simple starting conditions with visible physical interpretation should be related to these. Recently, speeding up of breeding has also become a perspective and actively developed application of dynamic models.

An imitation model as an instrument of hypothesizing and phenomenon interpretation. *Model interpretation of abnormal productivity functions.* One of the most known classic problems of agrochemistry discussed for more than 150 years but still important remains the determination and formalization of crop productivity response to external factors, in particular, to the dosages of introduced fertilizers [5]. Most often smooth unimodal curves or saturation curves are used for approximation of this dependence, which is completely compliant with the effects of increasing dosages of ecological factors (Liebig's and Shelford's laws). At the same time, in open sources one can often encounter a mention that the processing of obtained experimental data has led to identification of a more complex and, importantly, non-monotonous productivity function (further herein only the effect of nitrogen fertilizers would be referred to). In the area of the average values of the affecting factor, there is a trend to an intermediate plateau of the response function or even an intermediate breakdown occurs, and with increased dosages, yield increase is again observed, according to the expected standard trend [12-16].



**Fig. 1. Model functions of wheat productivity depending on nitrogen fertilizer dosages with "intermediate plateau" effect:** A — AGROSIM model (Leibniz Centre for Agricultural Landscape Research, Germany), B — AGROTOOL (Agrophysical Institute, Russia).

It is not very easy to unambiguously and simply explain the intermediate plateau or intermediate breakdown effect. In the joint study initiated by the authors, an attempt was made to use the calculations according to alternative dynamic models of the production process for spring wheat, AGROTOOL [17], and winter wheat, AGROSIM [5], in order to identify the described effect and to give a model interpretation to it. It was successful for both models (Fig. 1); the explanation of non-monotonousness of the obtained productivity function appeared to be different, although the required conditions of reproducibility for the described case for both models were similar (the presence of drought, i.e. a stress period of plant development preceding flowering) [17]. A principal factor in the AGROSIM model developed by specialists of Leibniz Centre for Agricultural Landscape Research (ZALF, Germany), was a partial translocation of structural biomass of roots and sprout in order to provide for energy to support

breathing. Such a phenomenon is observed in the model for medium dosages of pre-sowing fertilizer administration only, because at lower dosages the low value of structural biomass accumulated to the beginning of stress period does not form critical requests for breathing support while at large dosages these effects are covered by the present spare carbohydrate pool. In the AGROTOOL model, the same effect unclearly follows from the formalization of the carbon-nitrogen relationships in the plant realized therein [18].

In accordance with the proposed modeling method [6], the mechanism controlling the distribution of primary assimilates between sprouts and roots (growth functions) is an adaptive algorithm of balanced, i.e. most effective, growth of organs generating N and C, the main substrates for structural compound synthesis during vegetative ontogenesis in a double-stream system with spare metabolite pools.

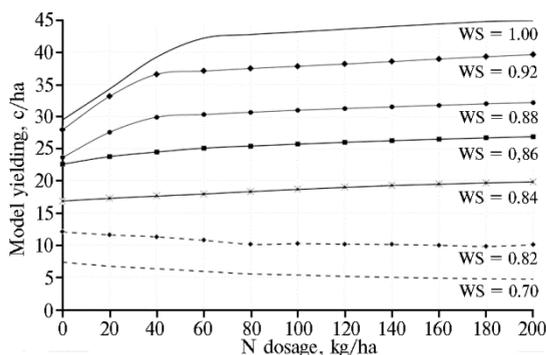
*Timing and microdosing effects in controlling the nitrogen nutrients.* The AGROTOOL-based calculations in order to determine optimal timings and dosages of nitrogen nutrients for intensive Daria spring wheat variety in the field tests (Men'kovskii branch of the Agrophysical Institute) gave non-trivial and unexpected results. The calculation experiments in the number of cases demonstrated an unusually high sensitivity of the model to timings of the non-root application of nutrients. Thus, it appeared to be that at certain conditions a 3- to 5- day delay in the treatment, when compared to the reference date, can reduce yield by up to 60 % from the maximum possible level, whereas at "guessing" of the nutrition timing, the model yield sharply increased compared to the control variant even at relatively insignificant (small) dosages of the active compound. Such results could have been ascribed to model imperfection but such behavior is quite well compliant with the relatively widely known and published data of real field experiments [10, 11, 19] confirming significant effects of nutrition timings on the final yield and a possibility to considerably affect it by small fertilizer dosages (microdosing).

The development of a model, i.e. a possibility to trace the growth and development of a model plant "in the tuning mode" allowed for understanding the reasons of the described effects on the algorithmic level. Thus, the performed studies have led to a conclusion that the timing effect (e.g. a drastic reduction in the final productivity at selection of an unfortunate nutrition date) is indeed reproduced in the model at certain combination of several specific conditions (in particular, at insignificant but necessary nitrogen deficit in the soil during the entire vegetation growth). The detailed analysis has shown that the obtained results may be interpreted and naturally follow from the simple assumptions that are comprised in the sub-model of carbon-nitrogen interaction [6, 18]. Thereby, nitrogen nutrition prior to flowering has not only a quantitative but also qualitative effect, regularly affecting growth, which can be both substantially positive and drastically negative.

*Combined effect of water and nitrogen stress.* It is well known to specialists of practical crop research that at poor moisture supply, i.e. under drought conditions, the introduction of significant dosages of mineral fertilizers may lead to the reverse effect and negatively affect the final productivity of the sowing. This fact may be reproduced in computer experiments with mechanistic agroecosystem models, even if they do not comprise any special non-linear dependencies and mechanisms of combined effect of water and nitrogen stress, and also description of the salt status of the plant is completely ignored.

Thus, the said regularity was obtained at the processing of results of model calculations when analyzing and comparing the sensitivity of two alternative models, AGROTOOL [17] and MONICA [20] to the simultaneous and separate effect

of drought and nitrogen deficit. In order to do this, a multi-factor computer experiment has been planned and carried out in the APEX system, a special control shell for automation of multi-variant calculations and the agricultural crop production models [4].



**Fig. 2.** Effect of combined influence of water and nitrogen stress on spring wheat (calculation data according to the AGROTOOL model): WS — water supply.

The control of the water stress parameters was carried out using the module of imitation of the automatic watering system realized in the AGROTOOL model [18]. The example of the obtained results (Fig. 2) demonstrates that the plots of the response function (the dependence of the economic crop on the pre-sowing dosage of nitrogen fertilizers for different conditional moisture supply) appear to be not similar, not equidistant, and, moreover, they are principally different. Thus, under

strong water stress the final productivity of the sowing does not grow but falls with an increase in the dosage of the pre-sowing nitrogen introduction. A detailed study of the model algorithms allows explaining the observed effect within the scope of the main used hypothesis on the double-stream C-N control in the plant and the mechanisms of calculating the root penetration depth comprised in the model depending on the moisture content in the soil profile.

Perspectives of using the imitation models in information selection provision. One can hardly recite a more conservative field of agricultural biology than selection. The existing gap between the flow-balance approach to describing physiological processes in plants accepted in all classical agroecosystem models and breeding methods based on the analysis of the quantitative traits at the genetic level appears to be especially terminal. Nevertheless, as traditional agricultural genetics encounters a necessity of an adequate response to modern challenges, complex mathematical models of the production process begin to be seriously considered as a genetic investigation tool. Most of such challenges are associated with the observed global changes, firstly, with the climate change [21]. Already almost no one argues the expectance of a significant increase in the instability of future crop yields due to the growth in the frequency and intensity of extreme effects (such as temperature stress and droughts). A response may be to provide principally novel crop varieties, firstly grain crops [22]. One of unexpected but powerful means of accelerating traditional selection may be the instrumentation of imitation modeling of agroecosystems [23]. These studies are associated with the ideotype term [24-25] or an ideal variety, as accepted in the Russian literature [26]. An ideotype is a theoretical future variety capable of giving theoretically possible yield in accordance with the bioclimatic potential (essentially, a potential aim of selection).

The qualitative assessments of the perspectives of the ideal variety for scientific forecast of the plant state and its separate features at growing under the present conditions have proven to be working [27, 28]; however, all advantages of such an approach can be disclosed only in combination with application of imitation agrosystem models. Thereby, genotypic adaptation, which implies introduction of new traits in the variety, as expected, would be one of the most important future strategies at climate change, and the modeling of agroecosystems may serve as basis for assessment of biophysical potential of crops provided

by such adaptation [29]. As a whole, one can refer to two trends which were formed in modern studies of agroecosystem model application in agricultural ecology and selection. These are the determination of zones beneficial for already existing varieties taking into the account the significant dynamics due to the climate changes, and the justification of requirements to traits of new varieties adapted to the expected environmental conditions.

The first direction is illustrated by the papers [30, 31], which, in particular, show that certain barley genotypes may be promising for the predicted climate change. The authors have proposed the most beneficial zones for specific ideotypes having a combination of several key genetic traits (phenology, leave growth, photosynthesis, drought resistance and grain formation). R.P. Rötter et al. [29] have analyzed the studies reflecting the second trend. Their review describes the main limitations and limits of using imitation modeling for supporting selection of agricultural crops and also outlines examples of assessment and formation of grain varieties for expected conditions using modeling. The agroecosystem models are used for identification of traits required for future varieties [32]. In the Western scientific community, the use of imitation models for acceleration of selection process has already become practical. Based on the advanced biologization of existing models, works have been started for their adaptation for novel application fields. In Russia, this trend should also be activated.

Therefore, despite certain objective limitations for practical agronomy, the imitation agroecosystem model can and should be viewed as a real tool for formalization of knowledge about processes and effects determining growth and development of cultivated plants. Moreover, the production process models help investigators in the agricultural biology to accelerate a transition from passive accumulation of plant description data to the active control of knowledge about processes and effects in agroecosystems [33-36]. The international symposium "Crop Modeling for Agriculture and Food Security under Global Change" (Berlin, 2016) has clearly outlined achievements, set specific goals and determined perspectives of using the imitation modeling in agricultural biology. It was noted that models can be a driving force of progress in improving agricultural crops, being a unique instrument of analysis and determination of beneficial genotypes (G, genotype) and management methods (M, management) for specific soil and climatic conditions (E, environment) taking into the account the resources present [37]. Only modeling allows for effectively analyzing the full spectrum of the  $G \times M \times E$  combinations and provides a rational basis for development and testing of novel wheat ideotypes optimized for target agricultural landscapes and future climatic conditions. The next generation models should comprise the so-called genetic coefficients for modeling differences between hybrids (gene-based crop model) [38]. Genomic forecasting using agricultural crop models is capable of performing better than statistical methods using only genetic data [39]. The main direction of model development is associated with improvement in the  $G \times M \times E$  interaction.

Thus, it is expected that substantial biologization would mainly determine the development of mechanistic models of the production process of agricultural crops. Moreover, we believe that within the scope of this direction results of any field experiments should be used only for identification of models, not for building them. Thereby, in the first place one should use hypotheses about the essence and driving force of biological processes in plant. Due to realization of such ideal plan, the model becomes an instrument of producing new knowledge for studying the agroecosystem response to all possible effects including those which still cannot be reproduced in a field experiment (e.g. associated

with the climate change).

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