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Abstract. The role of dynamic crop models as an intellectual core of computer decision support systems in agricultural management increases significantly in recent time. However, the scope of model applications is often limited by short time scale i.e. crop simulation/forecasting is performed within a particular vegetation season. The use of dynamic models in long-term planning is still much less developed. This contribution presents the author's efforts in development and improvement of the integrated system of crop simulation «APEX-AGROTOOL» for its use as a tool of model-oriented analysis of land use environmental sustainability. Attention is paid to the modification of the existing software in order to provide an ability to simulate agro-landscape dynamics taking into account crop rotation effects.

Keywords: crop rotation · sustainable agriculture · generic crop simulator · computer experiment · multivariate analysis · simulation software

1 Introduction

Maintaining or even increasing the fertility of agricultural landscapes during their active agricultural use is one of the most important scientific problems in theoretical agricultural science. The importance of this issue has recently increased due to significant changes in land use. For example, the new energy-oriented agriculture needs scientific support in many aspects: choice of the proper cultures, choice of crop rotation scheme, choice of crop allocation in different spatial scales etc. The main problem is to bridge the gap between economic requests and scientific methodological support of sustainable land use. In recent years agricultural science reinforced the efforts to achieve agrolandscape environmental sustainability instead of maximum productivity [1]. The paper presents efforts for development and improvement of the integrated system of crop simulation «APEX-AGROTOOL» for analysis and investigation of alternative medium-term planning strategies in land use, taking into account the crop rotation influence on environmental sustainability and saving resources.

2   Material and Methods

The use of dynamic imitation models is well-known and wide-distributed modern tool in agroecology and crop production for analyzing, forecasting and decision support. Numerous benefits of this approach in comparison with statistical and regression models are:

- improved accuracy and approximation of the calculations by taking more factors into account;
- obtaining multiple results based on the wider range of variations of input data;
- results produced as distributions of indicators on probability samples of external conditions can be readily used in risk analysis;
- almost unlimited number of monitored indicators of the agroecosystem model (productivity, environment, fertility, etc.);
- reduced uncertainty of model calculations, etc.

All these advantages of dynamic models are the basis of their wide application to real-time forecasting and crop management in the short time scale (within a particular growing season) [2]. However, their use for long-term planning is still much less developed. Until recently, it was mainly caused by technical limitations such as computational efficiency or memory size. At present, however, due to the progress in hardware engineering as well as in information technologies, the most significant restrictions have been overcome. Thus the subject-oriented requirements have become the principal feature for the applicability of imitation models in mid-term forecasting in agriculture [3].

An appropriate solution requires adaptation of both the models and the computer simulation environment for fulfilling the relevant task requirements. First of all, it refers to the need for a full description of the changes during the long-term crop rotation [4]. The latter involves the following specific requirements to imitation model:

- Universal character of the simulation algorithm. It includes structural identity of the models for different cultures/cultivars, soil-climate conditions and technologies.
- Comprehensive sequence analysis. The model should fully take into account the influence of culture predecessors in all significant aspects such as decomposition of crop residues and changes in the agrochemical and the physical properties of the soil, symbiotic nitrogen fixation legumes, etc. [5,6].
- «Wintering» imitation. The model should be able to simulate abiotic processes in the agroecosystem (soil frost penetration and thawing, snowfall and snow melting etc.) during off-seasons period.
- Environmental orientation. The model should be able to estimate yield as well as the dynamics of various parameters of the sustainability, such as soil fertility indexes (humus content, carbon sequestration), energy-matter balance of the agrolandscape (emission of greenhouse gases, biogen transfer to water body), etc.

In addition, special software for planning and performing the computer experiments with the model must be developed to provide the following:

- Multivariate analysis of the studied crop model. It means multiple running of the model with different input data sets defined during preprocessing. Moreover, crop rotation research needs strong sequence of scenario execution.
- GIS interface or integration with GIS software for visualization of simulated results (economical as well as ecological variables) on a farm scale.
- Built-in tools of model information support for model-based forecasting (weather and field test databases, stochastic weather generator, etc.)

Only the existence of a comprehensive ecologically oriented crop model and a special software providing cyclical scheme of model computation (taking into account crop rotation) will solve the problem of analyzing long-term trends of indicators of soil fertility and other parameters of the environmental sustainability of agricultural landscapes. The above mentioned requirements to a «model-centric» computer system of analysis and decision making support in sustainable agriculture seem to be rigorous. Nevertheless, the prototypes of such a system have been developed. For example, DSSAT (leading solution for crop modeling in the USA) includes special application for crop rotation analysis that assess economic risks and environmental impacts taking into account irrigation, fertilizer management, climate variability and changes, soil carbon sequestration, and precision management [7].

Examples of successful DSSAT applications for crop rotation analysis and optimization of combination of crop residue and N application rate for sustainable production are also known [8,9]. One of the most known European solutions for model-based analysis incorporating mid-term planning in farm scale is LandCare-DSS developed in the Leibniz Center of Agrolandscape Research [10]. LandCare-DSS features includes an original cartographical interface, close connection with a built-in module of economic analysis and the usage of different type of crop simulators depending on the spatial resolution of the investigated problem: from simplified regression model YieldStat at regional level to dynamic crop model MONICA at farm or field level.

Integrated simulation environment «APEX-AGROTOOL» is, probably, the most advanced Russian product providing information support, planning and running of multivariate computer experiments in crop modeling. The system was developed in Agrophysical Research Institute (Saint-Petersburg) and consists of two main parts: dynamic crop model AGROTOOL [11] and the system of model multivariate analysis APEX [12]. The principal modifications which have been made in software for «APEX-AGROTOOL» system to satisfy the above mentioned requirements of long term environmental analysis of agroecosystem dynamics are presented further.

3   Changes in the AGROTOOL Software

The simulation algorithm of AGROTOOL can be written in the form of recurrent discrete expression:

$$\mathbf{x}(k+1) = \mathbf{f}(\mathbf{x}(k), \mathbf{a}, \mathbf{w}(k), \mathbf{u}(k)), \qquad \mathbf{x}(0) = \mathbf{x_0}, k = 0,1...T \qquad (1)$$

where $\mathbf{x}$ - vector of dynamic state variables; $\mathbf{a}$ - vector of constant parameters; $\mathbf{u}$ - vector controlled external impacts (agricultural technician); $\mathbf{w}$ - vector uncontrollable external impacts; k - the time step for the model (time step is equal to one day), $\mathbf{f}$ - the evolution operator (a logical essence of the simulation algorithm).

Thus, AGROTOOL model recursively computes the vector of values of the modelling characteristics of the agroecosystem in the next step of the calculation on the base of the vector from the previous step. The main technical feature of the current version of AGROTOOL software is that all the data necessary for the calculation are stored in the model operational database, which is a multi-sheet Microsoft Excel document. Moreover, the same Microsoft Excel document also stores a detailed simulation results in the form of the state vector model at each step for calculating $\mathbf{y}(k)=\mathbf{y}(\mathbf{x}(k))$. Another important feature of AGROTOOL is the universal character of the simulation algorithm, i.e. it is so-called *generic crop simulator*.

A special modification has been developed for sequential modeling of crop rotation using AGROTOOL. Now it uses data from the operational database, stored there during the previous stage of calculation (for the predecessor crop) to be used as initial state for the calculation of the next crop. A formal procedure to perform recalculation is following: $\mathbf{x}_0^{i+1}=g(\mathbf{y}^i(T))$. In turn, the results of this calculation can be used to generate the initial state of the calculation of the crop of the successor of the second order, and thus closes the next "round" of crop rotation.

To carry out model calculations within the crop rotation in the current version of AGROTOOL software, it is necessary to know the dry biomass residue (separately for aboveground and root parts), nodule nitrogen (if the predecessor culture is legume), the total mineral nitrogen content and the humus in the soil. These values are fixed at the end of the season for the predecessor crop and "frozen", i.e. do not change until the time of sowing of the next succeeding crops. In the future, it is planned to develop an algorithm to study the behavior of these characteristics for non-vegetation period (wintering), including a simplified description of the transformations of these variables.

4   Changes in the APEX Software

The APEX software can be considered as a versatile repository of external crop model descriptors. Its interface permits users to register its own crop model or model version. Also APEX provides a universal environment for the polyvariant model analysis. It means designing and preparation of a multivariate computer case study, performing the model runs in batch mode and applying advanced procedures of statistical
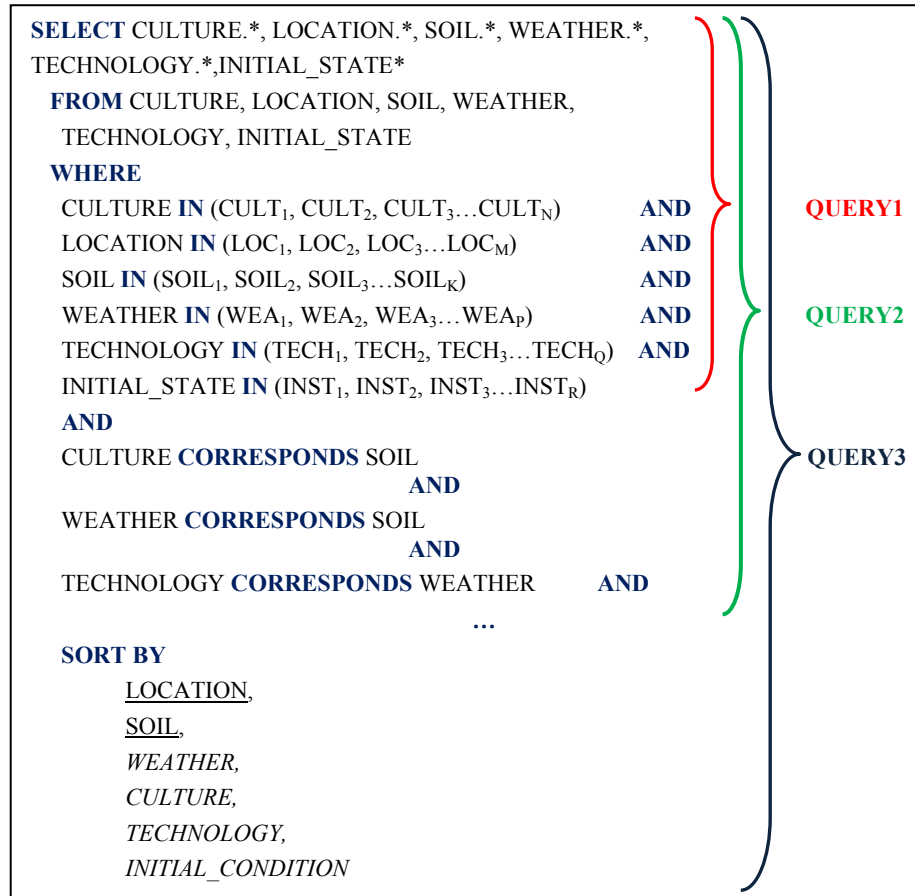
treatments for results obtained. Each set of input data forms a single scenario calculation. The scenario is a cortege of references to specific gradation of selected factors (information domain) specific to the subject area. These factors are following "soil", "culture", "area", "initial state", "technology" and "weather." During the registration of the model the software allows the user to specify the structure of variables and parameters for the specific model and to generate a list of tables and their fields, as well as an array of metadata. A more detailed description of the structure and principles of operation of the APEX software can be found in [12].

Rigid specification of the predefined factors enabled to perform "semantically rich" analysis of the results obtained using specialized software tools for preparation of input data (e.g. weather generator), although these features limit flexibility of the system. In particular, it allows implementation of the calculation of the crop rotations within the APEX software.

For automated calculation of crop rotations in APEX it is necessary to develop the following additional functionality:

- To implement a mechanism for the explicit specification of the sequence for the execution of scenarios in a framework of the project of computer experiment and to specify "boundary" scenarios, defining the beginning of the crop rotation block for a particular agricultural field.
- To create a flexible interface for specification the method for the "continuity" of the results of the previous scenario during the formation of the initial state for the next scenario (taking into account the "predecessor crop") in the procedure of the metadata specification describing the connected model.

The fundamental idea underlying the formation of an ordered list of scenarios in a structured polyvariant project calculation of crop rotation can be demonstrated by analogy with SQL-queries in a relational database (Fig.1). A simple project, realized by all possible combinations of all gradations of predefined factors (a full factorial experiment) in the framework of this analogy, can be represented by a QUERY1 (Fig. 1 – red), where the WHERE clause explicitly chooses the set of gradations for each of the predefined factors. The result of such query will be the Cartesian product of "all vs. all", generating $N * M * K * P * Q * R$ scenarios in a project.

```
SELECT CULTURE.*, LOCATION.*, SOIL.*, WEATHER.*,
TECHNOLOGY.*,INITIAL_STATE*
  FROM CULTURE, LOCATION, SOIL, WEATHER,
   TECHNOLOGY, INITIAL_STATE
  WHERE
   CULTURE IN (CULT₁, CULT₂, CULT₃…CULTₙ)          AND        QUERY1
   LOCATION IN (LOC₁, LOC₂, LOC₃…LOCₘ)             AND
   SOIL IN (SOIL₁, SOIL₂, SOIL₃…SOILₖ)             AND
   WEATHER IN (WEA₁, WEA₂, WEA₃…WEAₚ)              AND        QUERY2
   TECHNOLOGY IN (TECH₁, TECH₂, TECH₃…TECH_Q)      AND
   INITIAL_STATE IN (INST₁, INST₂, INST₃…INSTᵣ)
   AND
   CULTURE CORRESPONDS SOIL                                   QUERY3
                            AND
   WEATHER CORRESPONDS SOIL
                            AND
   TECHNOLOGY CORRESPONDS WEATHER       AND
                       …
   SORT BY
          LOCATION,
          SOIL,
          WEATHER,
          CULTURE,
          TECHNOLOGY,
          INITIAL_CONDITION
```

Fig. 1. Demonstration of the fundamental idea approach
(syntax does not coincide with the standard SQL)

Obviously, not all combinations of the factor gradations are meaningful. So it is clear that in a given year on the specific field only one crop involved in the crop rotation can grow. Thus, it is necessary to restrict the number of possible combinations and to form an incomplete factorial experiment scheme – QUERY2 (Fig.1 – green). Here, the second block of the AND clause is a set of additional links between the factor gradations. They are defined by the user in the specific APEX interface designed for the so-called "factor coupling".

A significant feature of the crop rotation project is the clear sequence of the execution of scenarios as results of the previous calculation can be used to generate the initial state at the next startup model in strict accordance with the scheme of crop changing. This is achieved by including a mechanism of the explicit specification of the order within factor gradations and between factors. The latter can be demonstrated by the introduction of sorting like QUERY3 (Fig.1 – blue).

The sequence of these factors in the SORT BY clause completely defines the scenario ordering within the project. The wizard dialog for creation of a new project for a simple "three-field - three-year" crop rotation scheme is shown in Fig. 2.
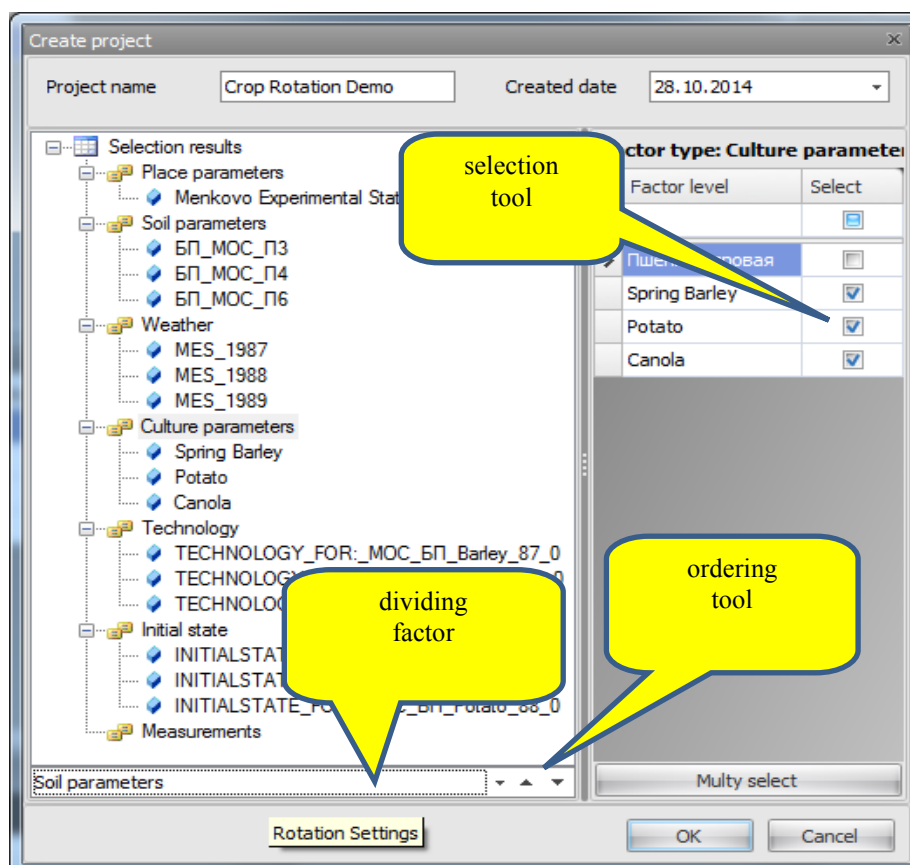
Fig. 2. The first step of the New Project Wizard

Fig.2 shows which factor used as a "separator" in the determination of the crop rotation (in this case, this factor is "soil"). As a result, a user can transparently specify the correct scenario order and define the boundaries of the "result continuity" blocks within simulated crop rotation. APEX performs the transfer of the results from the previously calculated variant to initial state of next variant inside every block following by the separating scenario. Thus, a set of scenarios, which make up the project, and a series-parallel scheme of their execution are fully defined. A typical interface with the project created in APEX is shown on Fig. 3.
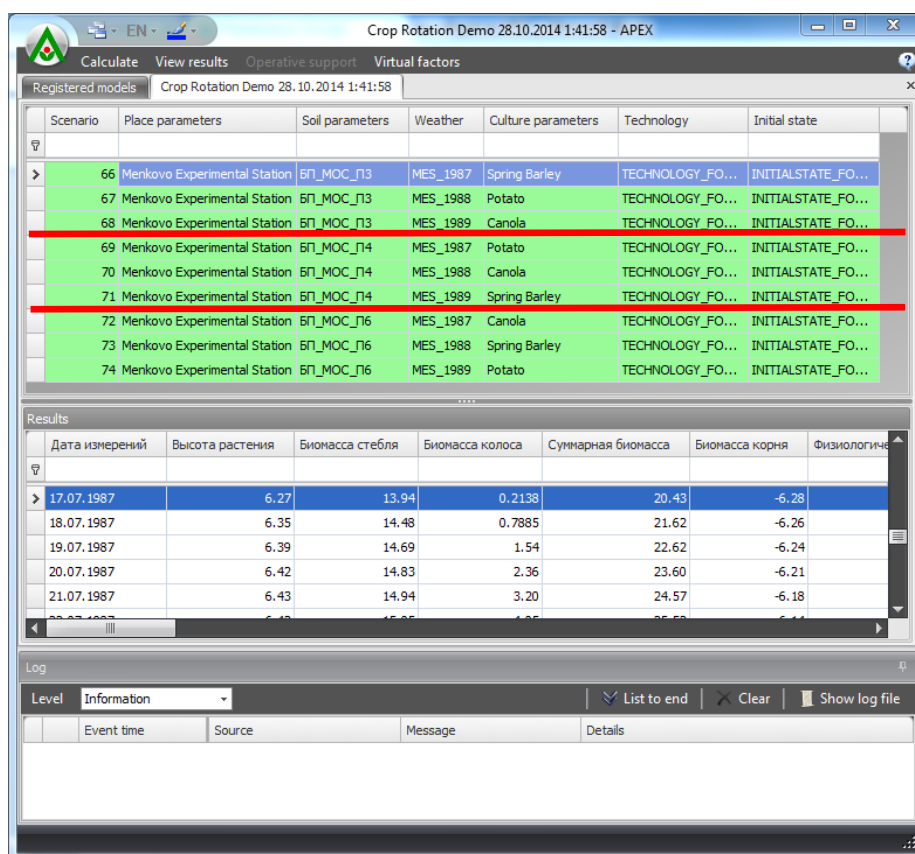
Fig. 3. Project visualization in APEX
(red line – the boundaries of the crop rotation logic blocks)

The method for transferring the results of the previous calculations into the certain fields of the gradation of the INITIAL_STATE factor for the next variant is described via a special APEX interface that is part of the input metadata about the connected models. Currently APEX supports two following modes: a) the selected INITIAL_STATE field can be directly equated to the value of selected calculation result and b) it can be declaratively assigned to a constant value. The latter method is used in conjunction as "environment APEX + model AGROTOOL».

5   Results

The degree of conformity of the achieved functionality of APEX and AGROTOOL with the above mentioned requirements of mid-term planning in land use is briefly summarized in Table 1. The abilities of the developed integrated environment cover

the needs completely and thus, the «APEX-AGROTOOL» system can be used as a tool of model-oriented analysis of land use environmental sustainability [13].

Requirement	Current state
Crop model:	**AGROTOOL:**
Generic simulator	Versatile algorithm for all maintained cultures. Calibrated models for cereals (summer and winter wheat, winter rye, barley, oats), maize, potato, root vegetables, annual and perennial forages, legumes.
«Wintering»	Continuous calculation. Modified descriptions of snow melting and soil thermal regime.
Predecessor influence	Separated calculation of litter and root residues in the module of carbon-nitrogen transfer and transformation in soil. Sub-model of symbiotic nitrogen fixation and nodule nitrogen dynamics.
Simulation infrastructure:	**APEX:**
Multiple running	Validated and implemented integrated environment for multivariate analysis and automation of computer experiments with crop models.
Crop rotation support	Special plug-in for planning not full factorial experiments and performing complex serial-parallel schemes of scenario computation.
Forecasting	Built-in stochastic generator of daily weather variables taking into account possible climate changes.

Table 1. Correspondence between mid-term planning requirements and abilities of «APEX+AGROTOOL» integrated software

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