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SPECIFIC CHARACTERISTICS OF THE APPLICATION OF MATHEMATICAL MODELING IN SOIL SCIENCE

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ABSTRACT: - The article talks about the use of mathematical modeling in the field of soil science. Empirical, semi-empirical, theoretical models are used in soil science, as well as their specific features. An overview, advantages and disadvantages of empirical, semi-empirical and theoretical models are analyzed. Necessary formulas and algorithms for mathematical modeling of heat transfer in the soil are compiled and their features are described.

KEYWORDS: Soil, mathematical models, empirical, semi-empirical, factor.

INTRODUCTION

At the intersection of several sciences, including biology, chemistry, physics, mathematics and cybernetics, a new science - mathematical soil science - has emerged and is developing. The development of mathematical models of the processes occurring in the soil structure is important not only in soil science, but also in the study of global processes in the biosphere [3].

Currently, the set of mathematical models known in soil science can be divided into 3 large groups: empirical, semi-empirical and theoretical models [7-8,11].

1. Empirical models. By observing the features of the object being studied in the construction of the models in this group, having a certain number of results depending on various factors of the external environment, the property of the soil being studied and its surroundings using the regression analysis

method gives rise to an analytical expression relating the features of the environment. Mathematical statistics is the study of various methods of processing multiple repeated random events and understanding their results.

Various functions with one or more variables are used in the construction of empirical models. In general, all empirical (regression) models can be written in the following form:

(1)

here - the studied feature of the environment, - environmental factors, - coefficients of the empirical model, - the total number of analyzed factors.

The numerical values of the parameters are obtained from the condition of the best match of the given theoretical and experimental (calculated according to formula (1)) values. In this case, the increase in the number of observations leads to an increase in additional data and an increase in the accuracy of smoothing [2]. In practice, in the process of measuring quantities, the values of almost always have random errors. To reduce (smooth) the effect of random errors, experiments are planned in such a way that the number of elements of the array of experimental data should be greater than the number of unknown parameters in model (1).

The disadvantage of these models is that they do not have the possibility to take into account causality and ecological hypotheses in the relations between variables. Also, in empirical models, the number of incoming indicators describing the actions of environmental factors ( ) is usually not large, so the accuracy of these models is not high. The most important drawback is that empirical models do not reveal the mechanism of the studied phenomenon, therefore, it is not possible to apply the model used in one condition to another condition different from this condition [1].

The most common types of nonlinear regression equations are: polynomial, hyperbolic, degree, exponential, binomial, logarithmic, trigonometric, logistic, etc.

After choosing the analytical representation of the function in the model (1) (this important step is called specific features of the model), the next step of modeling is the identification of parameters. If the function (1) is in the form of a degree polynomial, it is relatively easy to solve. In other more complex nonlinear cases, model linearization is resorted to. The selection of parameters of polynomial models is carried out by the method of least squares (EKKU).

There is an important class of models that linearize nonlinear variables using logarithmization and other similar transformations or numerical methods.

After determining the coefficients, the problem of calculating these coefficients and estimating the accuracy of the selected model in approximating the function (1) naturally arises.

Selection of the structure of empirical models (linearity, nonlinearity, etc.) and assessment of accuracy is carried out according to several criteria. Usually, the minimum of statistical indicators is taken as a criterion (correlation relationship or correlation index, mean squared error, average relative error of approximation between the values calculated according to the experimental and empirical model).

Regression equation (1) is divided into simple (even) and multiple regressions depending on the number of included factors.

Ordinal regression provides regression within and between. Commonly used empirical models are listed below:

In modeling, simple regression can give good results, if additional factors affecting the research object appear, multiple regression should be used.

Different types of functions containing one or more variables are used to study the relationship of productivity with agroclimatic, soil and agrotechnical factors. The main purpose of multiple regression is to create a model with a large number of factors, while determining the effect of each of them, as well as the total effect on the indicator being modeled.

Taking into account the exact interpretation of parameters, the most commonly used multiple regression types are: linear, parabolic, exponential, level, exponential-level, irrational, and others.

These models are listed below:

$$\tilde{y} = a_0 + \sum_{i=1}^{n} a_i \cdot x_i; \qquad \tilde{y} = a_0 + \sum_{i=1}^{n} a_i \cdot x_i + \sum_{i,j=1}^{n} a_{ij} x_i x_j;$$

$$\tilde{y} = a_0 + \sum_{i=1}^{n} a_i \cdot \sqrt{x_i} + \sum_{i,j=1}^{n} a_{ij} \cdot \sqrt{x_i x_j}; \qquad \tilde{y} = a_0 x_1^{a_1} x_2^{a_2} x_3^{a_3} \ldots x_n^{a_n}; \qquad (1)$$

$$\tilde{y} = a_0 e^{a_1 x_1 + a_2 x_2 + a_3 x_3 + \ldots + a_n x_n}; \qquad \tilde{y} = a_0 x_1^{a_1} x_2^{a_2} x_3^{a_3} \ldots x_n^{a_n} e^{b_1 x_1 + b_2 x_2 + b_3 x_3 + \ldots + b_n x_n}.$$

The parameters of linear multiple regression are called "pure" regression coefficients. They describe the average change of the result by changing the corresponding parameter by one, without changing the value of other factors.

Features of converting non-linear relationships into linear form, multiple regression parameters are also determined by EKKU, the only difference is that it is used not for the original data, but for the transformed data.

2. Semi-empirical models. Semi-empirical models differ from empirical models in that they are built on the basis of formulas that express the basic laws of nature. These laws can be the law of conservation of mass, the law of conservation of energy, thermodynamic equations of chemical balance, etc. [7]. These formulas are supplemented with empirical models of individual soil microprocesses, thus creating a "synthetic" model that describes the studied phenomena as a whole. But, as a rule, it is impossible to build a closed mathematical model of a complex natural system based only on equilibrium relations (laws of conservation), because the mechanisms of many processes occurring in them are not well studied, and the number of quantities always remains uncertain. To determine them, it is necessary to collect empirical data and process it with the methods of mathematical statistics. Therefore, this group of models is called semi-empirical.

Semi-empirical models are widely used in soil science. Based on the purpose of their composition, it opens up the possibility of combining our knowledge about the original system into a single whole, translating it into a single mathematical language and using it to solve various problems.

3. Theoretical models. Theoretical models differ from empirical (regression) models primarily by the amount of a priori data required for their construction. In empirical models, initial (theoretical) data are used only to select environmental factors, whose influence on the system is considered in the model.

However, the extreme complexity of soils and the lack of sufficient knowledge of the mechanisms of many soil processes hinder the development of this group of models. Theoretical modeling requires fundamental research.

The advantage of semi-empirical and theoretical models is the invariance of the initial formula representing the conservation law. Another advantage is the ability to calculate the detailed distribution of the studied process over time and soil layers. The weakness of semi-empirical and theoretical models is that it is not guaranteed that the model includes descriptions of all soil processes necessary for the occurrence of the considered phenomenon [4].

We have familiarized ourselves with various approaches to modeling soil processes, now we will move on to consider mathematical models of specific soil processes.

4. Mathematical modeling of heat transfer in soil. In soil science, much attention is paid to the modeling of heat exchange, because it has a significant impact on the speed of processes taking place in the soil structure, climate and ecosystem productivity. Description and solution of various problems of heat transfer in soils are considered in [1-4]. So, in order to solve the direct problem of heat transfer in the soil (prediction of the thermal conductivity in the soil) and the reverse problem (determining the heat diffusion according to the data of field or laboratory experiments), the classical heat transfer in the soil was studied:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}\left(\kappa = \frac{\lambda}{c_v}\right), \qquad (2)$$

where - the temperature of the soil at the point and moment of time, - heat transfer coefficient, - volumetric heat capacity of the soil, - density of the soil, - specific heat.

A one-dimensional unsteady heat transfer equation was studied in detail in [3] to account for the effect of filtration on changes in the thermal field of the soil aeration zone associated with changes in soil surface temperature:

$$\left(c_m \rho_m\right)\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_m \frac{\partial T}{\partial x}\right) \pm \left(c_f \rho_f\right)\frac{\partial\left(q_x T\right)}{\partial x}, \qquad (3)$$

where - coefficient of thermal conductivity, - volumetric heat capacity of the soil, - density of the soil, - specific heat, - heat capacity of a unit mass of water, - water density, - filtration rate, - water movement in the soil average speed, - the total porosity of the soil.

Based on the solution of equations (6) and (7), it is possible to create formulas for estimating point and average temperature at a certain soil thickness. In addition, a number of methods have been developed for quick and simple calculation of soil heat dissipation, taking into account the effect of surface temperature and the presence or absence of infiltration flow [4-6].

CONCLUSION

The article analyzes the mathematical models describing the processes occurring in the soil structure. The presented models require further theoretical and experimental research for various soil conditions.

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