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Determination of model parameters of water-nutritional processes in soil for nitrogen compounds

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Abstract. Studies of development of an integrated model that allows calculating the whole range of processes necessary for predicting and managing the water and nutrient regimes of reclaimed soils are considered. Calculated values of the maximum concentrations of nitrate nitrogen in the topsoil during the growing season of plant for Tashkent's region are shown. Values of field moisture capacity and wilting moisture of the main varieties of irrigated soils are defined.

1. Introduction

Intensification of agricultural production requires improved forecasting and management of water and nutrient regimes in soils [1, 2]. The moisture content of the soil determines the evaporation, transpiration of plants, being a key factor in the cycle. Soil solutions carry a significant amount of dissolved substances [3, 4].

Adequate description of the movement of water and nutrients in arable and arable zones is of great importance for the management of plant growth factors [5]. As the analysis of the most well-known models of moisture, mass transfer and development of agricultural crops [6-8] shows, at present there is no single software package that allows modeling the entire set of physical, biological and chemical processes in the zone of aeration and complete saturation, typical for reclaimed lands. Each specific model solves its highly specialized problem [9]. In some cases, the researcher is faced with the task of carrying out complex calculations and forecasts. In this case, it is necessary to reconcile various models, which is rather laborious and not always possible [10]. Therefore, the development of an integrated model that makes it possible to calculate the entire range of processes necessary for predicting and managing the water and nutrient regimes of reclaimed soils is a timely and urgent task [11].

In recent years, there has been a tendency to combine existing models of individual processes of moisture movement [12], transport and transformation of chemical compounds in soils into complex models [13] designed to describe soil regimes, which in some cases can be combined with models of moisture and chemical compounds movement in plants and ground air [14].

The choice of the model is due to its ability to calculate the nutrient regime and soil moisture in a one-dimensional formulation, taking into account the moisture intake by plant roots.

The methodology includes the following steps [15]:

1. The choice of calculation options, including the option with actually implemented water and nutritional regimes.

2. Calculation by the integrated model of water and nutrient regime for options.
3. Analysis of options, and selection of scenarios
4. Justification of the optimal option. As the optimal option, the one is chosen where the maximum crop yield was formed.

2. Research Methods

The scheme of the algorithm for calculating the model of processes in soil is as follows. At the first stage, for each specific year with a time step of one day, the potential total water consumption of plants is calculated. Then, for the same year, the actual components of the water balance are determined (evaporation, transpiration, etc.). For each day, according to the model of the aeration zone, the total water consumption of plants, the potentials of soil moisture in the aeration zone, the growth and development of plants, the transfer and transformation of nitrogen compounds are calculated [16]. This cycle is repeated for every day of the simulated period. To simulate the transfer and transformation of nitrogen compounds, the soil temperature is calculated, the decrease in decomposition coefficients depending on temperature, humidity, soil pH and the presence of oxygen, the transformation and transfer of organic nitrogen,

As noted in [17], the parameters of mass transfer are actually functions of the mass concentrations of the components, as well as temperature. In practical work, the form of these functions is set, and the constant coefficients, i.e., parameters are selected according to experimental data by optimizing the response variable [18].

To determine the parameters of the moisture conductivity model, the following data are needed [19]:

i) information about changes in humidity (or moisture potential) over time at several - at least two or three - depths inside the calculated layer;θ

ii) information about the change in time of the flow of moisture, moisture content or moisture potential at the boundaries of the calculated layer;

iii) values of moisture content or moisture potential along the entire profile of the calculated layer;

iv) water retention curves - depending on for each layer;θ

v) taking into account the development of plants during the measurement period - a model for calculating root water consumption.

The processes in the soil per unit volume of soil are as follows [20]

$$\Delta M = Q(z - \Delta z) - Q(z + \Delta z) - B(z) \quad (1)$$

which, in a one-dimensional dimension, reflects the change in the mass of the component with the cross-sectional area of the soil due to, respectively, the inflow through the upper and outflow of the lower edge of the balance volume Q along the coordinate at the mass of the transformed (produced) component $B(z)$.

In the liquid phase the differential equation for the conservation of the mass of a nutrient (in this case, nitrate nitrogen NO_3)

$$\frac{\partial\theta}{\partial t} = -\frac{\partial}{\partial z}\left[k \cdot \frac{\partial}{\partial z}(\psi + z)\right] - R \quad (2)$$

here $\theta -$ the volumetric soil moisture, $m^3 \cdot m^{-3}$; ψ - plant suction pressure, mm;

R - loss of substance as a result of transformation, in this case nitrate nitrogen as a result of denitrification.

For a model that implements the model of moisture transfer, it is possible to set a mode of outputting results that allows one to obtain the calculated values of the potentials (or moisture values) at the same depths where the measurements were carried out and at the same times when they were carried out. Based on these data, it is possible to calculate the values of the response variable corresponding to the set of values of the moisture conductivity parameters selected for the calculation. In the course of repeated calculations of moisture transfer, the desired parameter values can be found. Then it is required to check the adequacy of the moisture conductivity model by introducing additional parameters, or to change the model formula.

In the liquid phase, the differential equation for the conservation of the mass of the nutrient (in this case, nitrate nitrogen NO_3)

$$\frac{\partial\theta}{\partial t} = -\frac{\partial}{\partial z}\left[k \cdot \frac{\partial}{\partial z}(\psi + z)\right] - R \quad (3)$$

here θ - bulk soil moisture, $m^3 \cdot m^{-3}$; ψ - plant suction pressure, mm; R - loss of substance as a result of transformation, in this case nitrate nitrogen as a result of denitrification.
When calculating moisture transfer, which must be carried out when modeling the transfer of any components in soils, the transfer parameters according to [7] are the functions shown in Figure 1.

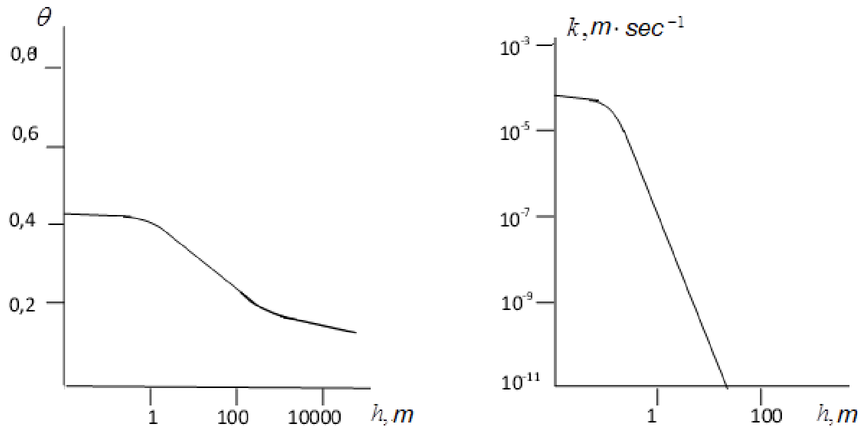

Figure 1. Dependences of moisture content and moisture conductivity coefficient on suction pressure in loamy soils

To solve the equations of moisture transfer, we use the finite difference method. According to the data in Fig. 1, simple empirical models can be adopted for the given dependences

$$k = b_1, \theta = b_2 - b_3 \cdot k$$

here $b_1, b_2, b_3 -$ constants.

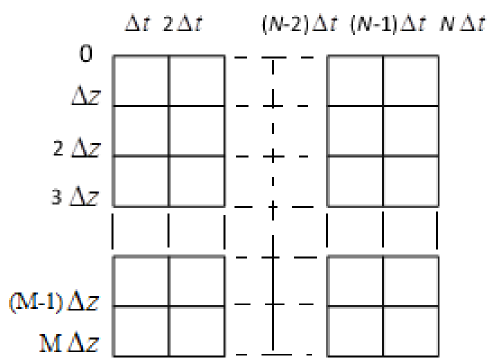

Figure 2. Grid for the numerical solution of the equation of the moisture transfer model

In this case, the equation is on the form

$$\frac{\rho}{\rho_w} b_3 \cdot \frac{\partial h}{\partial t} = b_1 \cdot \frac{\partial^2 h}{\partial z^2} \tag{4}$$

here ρ_w, ρ - the densities of the solution and soil.
There was considered the depth interval $z$from 0 to L and the time interval from 0 to t_k. According to the developed method, the model equation is replaced by a system of balance equations for layers of finite thickness. The value Δz is the step along the spatial coordinate, and Δt is the time step (Figure 2).

To find an approximate solution to equation (4), the differential equation is replaced by a system of simpler algebraic equations, in which the values in our case h are determined at the grid nodes. For this, the derivatives are replaced by differences and finally

$${}_{m,n+1} = \alpha \cdot h_{m+1,n} + (1 - 2 \cdot \alpha) \cdot h_{m,n} + \alpha \cdot h_{m-1,n}$$

here $\alpha = \Delta t \cdot b_1 \cdot \rho_w / (\rho \cdot b_3 \cdot \Delta z^2)$

For soil layer depth 0.3 m the initial equilibrium distribution of the suction pressure along the profile corresponds to the formula $h = 0{,}8 - z$, provided that at the upper end $z = 0$. Initial data for calculations according to Fig. 1

$$b_1 = 5 \cdot 10^{-5} m \cdot sec^{-1}, b_2 = 0{,}42 \kappa g/\kappa g^{-3}, b_3 = 0{,}1575 m^{-1}, \Delta z = 0{,}1 m, \Delta t = 0{,}4 sec$$
$$\rho = 1{,}5 \cdot 10^{-3} kg/m^{-3}, .\rho_w = 1{,}0 \cdot 10^{-3} kg/m^{-3}$$

Models describing mass transfer in soils should be supplemented with models for finding fluxes at boundaries. The soil surface is taken as the upper boundary of the calculated layer, where $z = 0$ the position of the lower boundary is different.

The surface evaporation model includes the amount of potential evaporation E, a correction for vegetation cover β, and a correction for topsoil moisture B. The density correction depends on the phase of plant development.

$$q = E \cdot \beta \cdot B \quad (5)$$

Observations of meteorological stations provide only data on temperature and air humidity. They can be used to calculate the monthly average values of the intensity of potential evaporation according to the formula [19]

$$E = 6{,}94 \cdot 10^{-9} \cdot (T - 248)^2 \cdot (100 - a) \quad (6)$$

a - lack of moisture in the soil.

Because rainfall in the period from mid-May to mid-October on the territory of the republic is insignificant, then the water supply of plants is due to irrigation. Evaporation of moisture from green leaves (transpiration) is an important physiological process, due to which water exchange in plants is ensured, a continuous flow of water with dissolved nutrients is created from the roots to terrestrial organs and leaves.

Young leaves evaporate more water than old ones. One and the same sheet from the lower surface evaporates water 2.5 ÷ 4.0 times more than from the upper one. One plant during the growing season (cotton, corn, sunflower) spends about 170÷190 liters of water on transpiration. The transpiration coefficient (Kt) of cotton is 645 (water consumption in grams to create one gram of dry mass) [20].

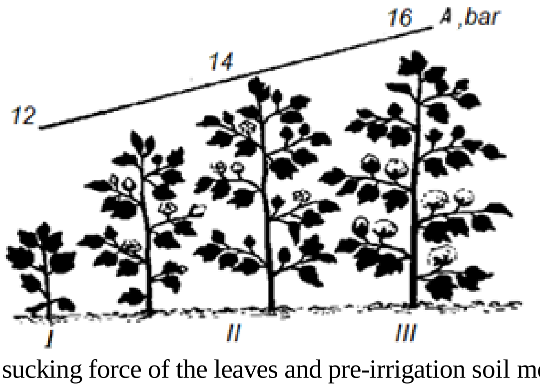

Figure 3. The value of the sucking force of the leaves and pre-irrigation soil moisture in cotton: I. From germination to flowering (75% of the irrigation rate); II. Flowering – fruiting (70% of the irrigation rate); III. Maturation (65% of the watering rate)

During transpiration, each cell or whole organ of the plant with a certain force takes and retains water, which creates a sucking force in the plant, with the help of which the evaporation of water through the leaves is compensated for by its absorption through the roots. The absorption of water and its rise up the plant is carried out as a result of the combined action of two factors: root pressure and the suction force of the leaves, which is formed during transpiration.

3. Results

Field experiments have established that the higher the temperature, the higher the rate of growth processes. The highest growth rate of the main stem is in cotton in May and especially in June crops. With late sowing, due to high average daily temperatures, the main stem is stretched. On early sowing, plant growth is more restrained, they have more fruit branches and fruit organs, the root system is more developed, since the development of cotton takes place in different conditions of temperature and illumination than at late sowing terms. The amount of incoming water is directly related to the development (capacity) of the root system. The values of field moisture capacity and wilting moisture of the main soil varieties of irrigated soils are given in Table 1.

Table 1. The values of field moisture capacity and wilting moisture of the main soil varieties of irrigated soils (% to the weight of the soil) [20]

Gray soil	Field moisture	Wilting moisture	Gray soil	Field moisture	Wilting moisture
Heavy loamy	22	10	Heavy loamy	24	12
Medium loamy	19	8	Medium loamy	21	9
Light loam	16	6	Light loam	18	7

Transforming these figures, one can move on to more understandable indicators of soil moisture reserves, expressed in m^3/ha (Table 2).

Table 2. Moisture reserve in a meter layer of soil (m^3 / ha) from mechanical composition

The soil	Moisture reserve or irrigation water capacity (100 %)	Permissible decrease in soil moisture (70%)	Moisture deficiency or field rate (30%)
Heavy loamy	3190	2233	957
Medium loamy	2870	1946	834
Light loamy	2320	1624	696

Subtracting from of the existing moisture reserves (at 100% field moisture capacity), the amount of water with a decrease in soil moisture to 70% (after which wilting begins), we can roughly determine the moisture deficit or the size of the next irrigation rate in m^3 / ha.

The general view of the change in the control concentration of nitrogen compounds in the soil during the period of plant development is shown in Figure 4, which makes it possible to further determine the need for nitrogen fertilizers.

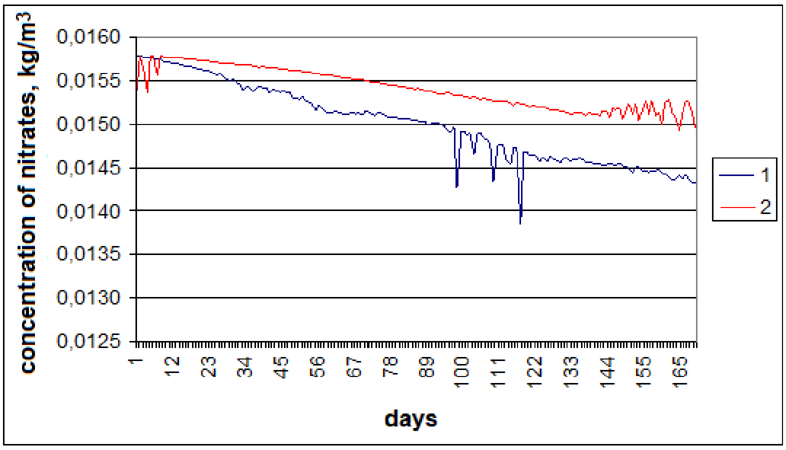

Figure 4. Calculated values of the maximum concentrations of nitrate nitrogen in the topsoil during the growing season of plant development. Legend: 1 - for standard moisture capacity, 2 - for moisture content 0.7 irrigation rate

4. Conclusions

Verification examples included the following tasks: moisture transfer taking into account crop cultivation and irrigation; migration and transformation of nitrogen compounds taking into account all simulated processes. The maximum deviations in the verification of the moisture transfer model, excluding problems for extreme conditions, were no more than 4%. The maximum deviations in the verification of the model of migration and transformation of nitrogen compounds were no more than 8%. This confirms the rather high degree of similarity of the results.

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