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# Predicting the scanning branches of hysteretic soil water-retention capacity with use of the method of mathematical modeling

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# Predicting the scanning branches of hysteretic soil water-retention capacity with use of the method of mathematical modeling

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**Abstract.** A mathematical model of the hysteresis of the water-retention capacity of the soil is proposed. The parameters of the model are interpreted within the framework of physical concepts of the structure and capillary properties of soil pores. On the basis of the model, a computer program with an interface that allows for dialogue with the user is developed. The program has some of options: visualization of experimental data; identification of the model parameters with use of measured data by means of an optimizing algorithm; graphical presentation of the hysteresis loop with application of the assigned parameters. Using the program, computational experiments were carried out, which consisted in verifying the identifiability of the model parameters from data on the main branches, and also in testing the ability to predict the scanning branches of the hysteresis loop. For the experiments, literature data on two sandy soils were used. The absence of an "artificial pump effect" is proved. A sufficiently high accuracy of the prediction of the scanning branches of the hysteresis loop has been achieved in comparison with the three models of the precursors. The practical importance of the proposed model and computer program, which is developed on its basis, is to ensure the calculation of precision irrigation rates. The application of such rates in irrigation farming will help to prevent excess moisture from flowing beyond the root layer of the soil and, thus, minimize the unproductive loss of irrigation water and agrochemicals, as well as reduce the risk of groundwater contamination and natural water eutrophication.

## 1. Introduction

The study of the hydrological conditions of the territory is an important part of engineering research in the substantiation of pre-design solutions in land reclamation. The data of these studies are of great importance for performing technological calculations during the exploitation of ameliorative systems.

The availability of reliable information on the hydrophysical properties of the soil is a prerequisite for achieving high accuracy of engineering and technological calculations. Among the most important indicators characterizing the hydrophysical properties of the soil, its water-retention capacity (WRC) refers. This indicator is usually described as a dependency of the volumetric water content θ [$cm^3 \cdot cm^{-3}$] on the capillary pressure of soil moisture ψ [cm $H_2O$]. Because of the hysteresis phenomenon the WRC curves, obtained by the measurements of soil drying, do not coincide with the soil wetting curves. The WRC direct measurement is a rather laborious process. Taking into account the multiplicity of the scanning branches filling the WRC hysteresis loop, a direct measurement of this indicator is an almost insoluble problem. The only alternative to direct measurements is the method of mathematical modeling.

In this paper, a mathematical model of the hysteretic WRC is proposed, substantiated within the framework of physical concepts of the structure and capillary properties of the soil pore space. The purpose of the work is the verification of the proposed model on the experimental data from the literature sources, as well as the comparison of the model with known analogs. As a comparison criterion, the error of prediction of scanning branches is used using some models whose parameters are estimated from data on the main branches of the WRC hysteresis loop. Such an indicator is the average absolute deviation of the simulation results from the experimental data.

## 2. Materials And Methods

In irrigation farming, the availability of the WRC data is the most important condition for calculating the irrigation rate. The simplest (but insufficiently accurate) method of this calculation is based on the use measured WRC data about the main drying curve (MDC). This curve is usually measured by the press method, successively displacing the water with pneumatic pressure from previously moistened soil samples. On the curve obtained by this method, a number of special points separating the intervals of qualitatively different states of soil moisture are distinguished. The values of volumetric soil water content corresponding to these points are called soil-hydrological constants (SHC). Such constants include: the saturation capacity (SC), the field capacity (FC), the moisture of capillary break (CB), the moisture of permanent wilting point (WP), the maximum hygroscopy (MH). Usually units of measurement of volumetric water content are used as units of SHC. The indicated SHCs characterize: SC - the maximum specific volume of water as a liquid in the soil; FC - the maximum specific volume of moisture retained by the capillary sorption forces of the soil; CB - boundary between the category of easily available water for plants and the category of difficultly available water for plants; WP - border, on which irreversible loss the plant turgor occurs; MH - is the minimum specific volume of water as a fluid in the soil. The difference FC-WP characterizes the reserve of productive moisture in the soil.

In practical irrigation farming, the irrigation rate is often calculated by the difference in FC -CB or by the difference between FC and the volumetric water content in the soil before watering. With this approach, a methodological error is quite obvious. Indeed, FC and CB are determined by the main drying branch, however, in watering, the change of moisture states in the soil is described not by the drying, but by the wetting branch. For this reason, the irrigation rate is surely overestimated. This error is explained as follows. The ability of the soil to retaining the water is determined not by the moisture reserves, but by the capillary pressure of soil moisture. In other words, if, when watering, the volumetric water content reaches a value that corresponds to FC, this does not mean that soil moisture does not flow off the root layer. According to the physical concepts of the nature of the WRC, moisture is in the soil in a capillary-suspended state, until the negative capillary pressure exceeds the value that corresponds to the FC.

The peculiarity of the hysteretic soil WRC is that the primary wetting curve (PWC), which starts from a certain reversal points on MDC, is always located below MDC. This means that with the same moisture reserves under wetting and drying conditions, the capillary pressure values differ: at the volumetric water content equal FC, the capillary pressure for the wetting curve reaches a higher value than for MDC. Thus, if the initial volumetric water content is equal to the CB, then under the rate of the FC-CB the soil achieves moistening status equal to FC, but the capillary pressure value is higher than the value corresponding to the FC measured at the MDC. As a result, excess free moisture flows under the action of gravity beyond the root layer. The authors do not propose in this article to prove the negative nature of the consequences of applying excessive irrigation rates (unproductive loss of the irrigation water, removal of nutrients and other agrochemicals into groundwater, etc.). It is important here to identify the problem and suggest ways to solve it.

Probably, this problem can be solved by using in the calculation of irrigation rates a predetermined and measured WRC wetting branch. We can partially agree with this assumption if irrigation farming is carried out in conditions that are protected from atmospheric precipitation. In fact, having measured data on the wetting branch from some fixed point (for example, CB) to FC, one can periodically apply the same irrigation rate calculated from the difference FC-CB. However, such a technique is not without drawbacks because when oscillating capillary pressure in a certain fixed interval, some drift of the volumetric water content values may occur in the range limited by the main branches of the WRC hysteresis loop. This is a natural phenomenon. In this case, a series of measurements of the scanning branches corresponding to each new oscillation will be required.

If we assume that the oscillation process is rapidly converging to some conditionally stable internal WRC hysteresis loop, then it would be possible to confine ourselves to a small number of measurements. However, as already noted, the direct WRC measurements are rather laborious, so even a relatively small increase in the volume of measurements leads to a significant reach in costs.

If the cultivation of crops is carried out in natural conditions, at the beginning of the rain, the soil moisture shifts from the states described by MDC to the states described by the PWCs, which start from reversal points whose positions are not known in advance (the probable feature of the weather forecast). The end of the rain leads to the transition to the secondary drying curves from the turning points, the positions of which are also not known in advance. Hence, it becomes obvious that in order to take into account possible scenarios for atmospheric moistening of the soil, an unlimited raw of measurements of the scanning branches of the WRC hysteresis loop will be required, which is practically impracticable. Thus, the only possible method of obtaining an exhaustive volume of data on the hysteretic soil WRC is the method of mathematical modeling.

In this paper, the literature WRC data on two sandy soils are used: white silica sand [1] and dune sand [2]. To describe the hysteretic hydrophysical properties of these soils, four models suggested by Scott and co-authors [3], Kool and Parker [4], Huang and co-authors [1] as well as by authors of this article are used.

Theory:

The concept of pore size distribution, as well as capillary phenomena in the pore space, is very productive in modeling the hydrophysical properties of the soil [5]. Following Kosugi [6-8], to describe the WRC, the authors of this paper use the function [9-12]:

$$S_e = \begin{cases} \frac{1}{2}\operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4}\ln\left(\frac{\psi-\psi_{ae}}{\psi_0-\psi_{ae}}\right)\right), & \psi < \psi_{ae}; \\ 1, & \psi \ge \psi_{ae}, \end{cases} \quad (1)$$

where: $S_e = (\theta-\theta_R)/(\theta_S-\theta_R)$ – effective saturation; $\theta_S$ [см$^3$·см$^{-3}$] - saturated volumetric water content; $\theta_R$ [см$^3$·см$^{-3}$] – residual volumetric water content; $n = 4/(\sigma\sqrt{2\pi})$; $\psi_{ae}$ [см $H_2O$] – capillary pressure of soil moisture under air entrance condition (bubbling pressure); $\psi_0$ [см $H_2O$] – capillary pressure, which corresponds to the most probable value of the random variable - the logarithm of the effective radius of the soil pore, $\sigma$ - the standard deviation of this random variable; $\operatorname{erfc}(z) = 1-(2/\sqrt{\pi})\int_0^z \exp(-t^2)dt$ - the complementary error function.

In [13, 14], for the function (1) an approximation is proposed:

$$S_e \approx \begin{cases} \left(1+\left(\dfrac{\psi-\psi_{ae}}{\psi_0-\psi_{ae}}\right)^n\right)^{-1}, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}. \end{cases} \quad (2)$$

When $\psi_{ae} = 0$ function (1) is a model of Kosugi [7, 8], and the approximation (2) is reduced to the WRC model proposed in [15-17]. However, unlike the model proposed in [15-17], the parameters of the relation (2) are physically interpreted.

By definition, the antiderivative for the differential moisture capacity function $\mu = d\theta/d\psi$ is a function of the integral moisture capacity, which describes the WRC. In developing a hysteretic WRC model, the authors of this paper use the assumption that the function $\mu = d\theta/d\psi$ at each point on the branch of the hysteresis loop takes two (and only two) values that correspond to the sorption and desorption equilibrium of soil moisture. Therefore, two sets of parameters $\psi_{0,d}$ [cm $H_2O$], $\psi_{ae}$ [cm $H_2O$] and $n_d$ (for desorption equilibrium of moisture), as well as $\psi_{0,w}$ [cm $H_2O$], $\psi_{we}$ [cm $H_2O$] and $n_w$ (for sorption equilibria of moisture) are further used to describe the hysteresis of the soil WRC by means of the relation (2). The scanning (primary, secondary, etc.) branches of the hysteresis loop start from reversal points, the calculation algorithm of which was proposed by Scott and co-authors in [3].

The presence of parameters $\psi_{ae}$ and $\psi_{we}$ in formula (2) required the inclusion of refinement conditions in the algorithm. To describe the drying branch, starting from the i-th point on the wetting branch, the following formulas are used:

$$\begin{cases} \begin{cases} S_{e,d} = \left(1+\left(\dfrac{\psi-\psi_{ae}}{\psi_{0,d}-\psi_{ae}}\right)^{n_d}\right)^{-1}, \\ \theta = \theta_R + (\theta_S^* - \theta_R) S_{e,d}, \\ \theta_S^* = \theta_s, \ \psi_{we} \leq \psi_i, \ \psi < \psi_{ae}; \\ \theta_S^* = \theta_i, \ \psi_{ae} \leq \psi_i < \psi_{we}, \ \psi < \psi_{ae}; \\ \theta_S^* = \dfrac{\theta_i - \theta_R (1 - S_{e,d}(\psi_i))}{S_{e,d}(\psi_i)}, \ \psi_i < \psi_{ae}, \ \psi \leq \psi_i; \end{cases} \\ \begin{cases} \theta = \theta_s, \ \psi_{we} \leq \psi_i, \ \psi_{ae} \leq \psi \leq \psi_i; \\ \theta = \theta_i, \ \psi_{ae} \leq \psi_i < \psi_{we}, \ \psi_{ae} \leq \psi \leq \psi_i. \end{cases} \end{cases} \quad (3a)$$

To describe the wetting branch, starting from the j-th point on the drying branch, the following formulas are used:

$$\left\{\begin{array}{l}\left[\begin{array}{l}S_{\mathrm{e,w}}=\left(1+\left(\dfrac{\psi-\psi_{\mathrm{we}}}{\psi_{0,\mathrm{w}}-\psi_{\mathrm{we}}}\right)^{n_{\mathrm{w}}}\right)^{-1},\\ \theta=\theta_{\mathrm{R}}^{*}+\left(\theta_{\mathrm{S}}-\theta_{\mathrm{R}}^{*}\right)S_{\mathrm{e,w}},\\ \theta_{\mathrm{R}}^{*}=\theta_{\mathrm{j}}=\theta_{\mathrm{r}},\ \psi_{\mathrm{j}}<<\psi_{\mathrm{ae}},\psi_{\mathrm{j}}\le\psi<\psi_{\mathrm{we}};\\ \theta_{\mathrm{R}}^{*}=\dfrac{\theta_{\mathrm{j}}-\theta_{\mathrm{S}}S_{\mathrm{e,w}}\left(\psi_{\mathrm{j}}\right)}{1-S_{\mathrm{e,w}}\left(\psi_{\mathrm{j}}\right)},\ \psi_{\mathrm{j}}<\psi_{\mathrm{ae}},\psi_{\mathrm{j}}\le\psi<\psi_{\mathrm{we}};\end{array}\right.\\ \left[\begin{array}{l}\theta=\theta_{\mathrm{S}},\ \psi_{\mathrm{j}}<\psi_{\mathrm{ae}},\psi_{\mathrm{we}}\le\psi;\\ \theta=\theta_{\mathrm{j}}=\theta_{\mathrm{s}},\ \psi_{\mathrm{ae}}\le\psi_{\mathrm{j}},\psi_{\mathrm{j}}\le\psi.\end{array}\right.\end{array}\right. \tag{3b}$$

### 3. Results and Discussions

Based on the hysteretic WRC model, formulated by the relations (3*a*) and (3*b*), a computer program "Hysteresis" was developed, in which the branches of the hysteresis loop are calculated. Using this program, two computational experiments were carried out.

The first experiment was aimed at revealing the possible presence of undesirable "artificial pump effect" in the model. To do this, a "scenario" was set for varying the values of the capillary pressure in the range from 40 cm $H_2O$ to 120 cm $H_2O$. At the same time, the "input" to the specified range of capillary pressure was carried out both from the main drying curve (MDC) and from the main wetting curve (MWC). The calculation uses the parameters of relation (2), identified using measured data on the white silica sand [1]. Figure 1 shows the results of constructing a hysteresis loop for oscillating capillary pressure in a fixed range. Analysis of figure 1 indicates that there is no undesirable "artificial pump effect".

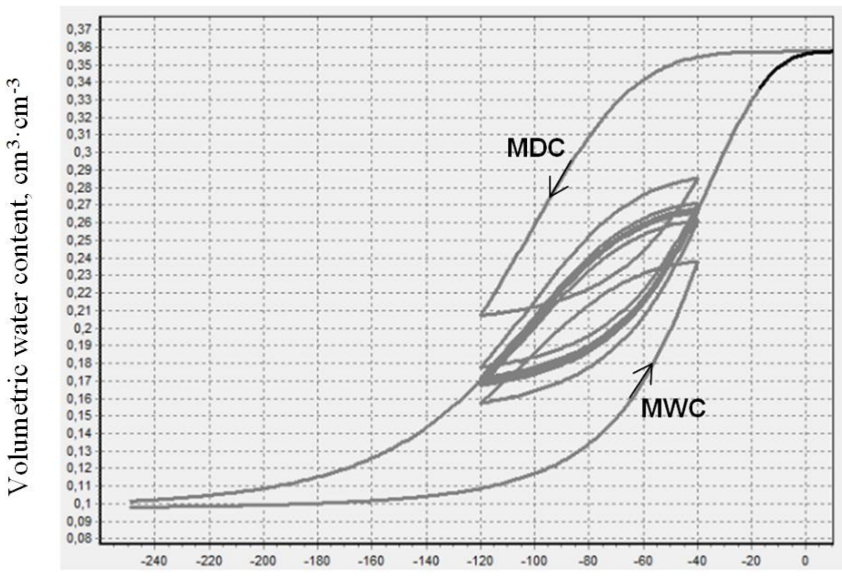


Figure 1. Sequence of the drying and wetting branches of the WRC hysteresis loop of the white silica sand [1] under oscillation of capillary pressure in a fixed range.

The second experiment was aimed at investigating the physical adequacy of the model underlying the "Hysteresis" program. The experiment consisted of several stages: i) identification of model parameters by fit-approximating the measured WRC data on the main drying and wetting branches of the investigated soils [1, 2]; ii) predicting the scanning branches of the hysteresis loop; iii) estimating the errors in the prediction of the scanning branches (the mean absolute value of the deviation of the calculation results from the experimental data); iv ) a comparison of the model proposed by the authors with the models by Scott and co-authors [3], Kool and Parker [4] as well as Huang and co-authors [1] using the error criterion.

On figure 2, as an example, a window of the program interface is shown, in which: red dots represent measured WRC data for the white silica sand [1]; in the upper left corner the parameters identified by fit-approximating the measured WRC data on the main branches; black diamond-shaped points connected by a solid curve, the results of fit-approximating the main branches are shown (directions are indicated by arrows), as well as the results of predicting the primary wetting branch, the secondary drying branch, and the tertiary wetting branch of the hysteresis loop.

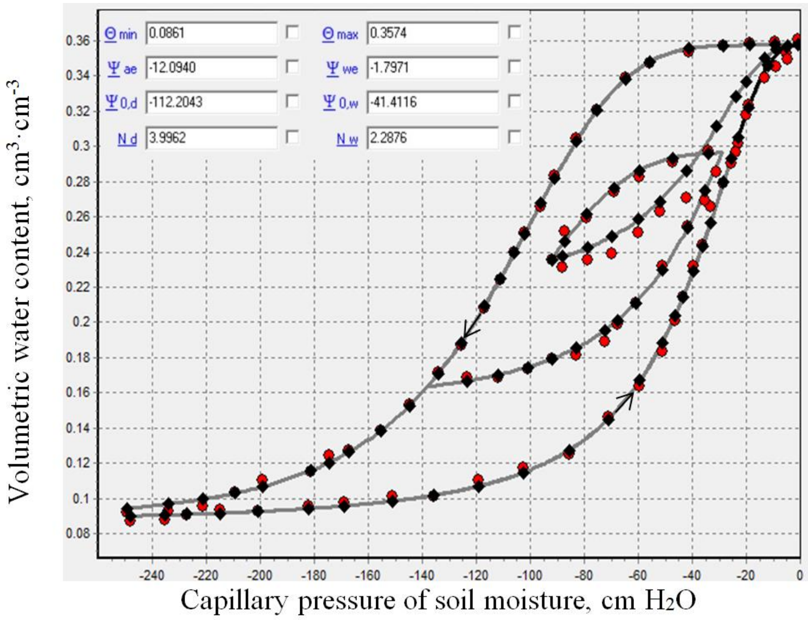


Figure 2. Identification of the parameters of the model proposed by the authors of the article, by fit-approximating of the measured WRC data on the main branches; prediction of the primary wetting branch, the secondary drying branch, the tertiary wetting branch of the WRC hysteresis loop of the white silica sand [1].

**Table 1.** Comparison of the four models by the error criterion the mean absolute value of the deviation of the simulation results from the measured data for the white silica sand [1]

| | Models | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | Scott et al. [3] | | Kool-Parker [4] | | Huang et al. [1] | | This paper | |
| Branches | Wetting | Drying | Wetting | Drying | Wetting | Drying | Wetting | Drying |
| Main | 0.0031 | 0.0026 | 0.0105 | 0.0108 | 0.0036 | 0.0025 | **0.0015** | **0.0023** |
| Primary | **0.0033** | 0.0070 | 0.0035 | 0.0028 | 0.0035 | 0.0066 | 0.0072 | **0.0024** |
| Secondary | 0.0029 | 0.0035 | 0.0054 | 0.0095 | 0.0050 | 0.0031 | **0.0028** | **0.0014** |
| Tertiary | 0.0099 | 0.0128 | 0.0130 | 0.0137 | **0.0082** | **0.0042** | 0.0149 | 0.0130 |

As can be seen from Table. 1, with respect to five of the eight investigated branches, the error of the model proposed by the authors of this article turned out to be lower in comparison with other models. It is necessary to pay attention to the tertiary wetting branches. The measured points on these branches intersect the main wetting branch of hysteretic loop. This "phenomena" cannot be explained from physical considerations; therefore the models by Scott and co-authors [3], by Kool and Parker [4], and also the model proposed by the authors of this paper, are characterized as comparable, but more "high" errors, in contrast with the model by Huang and co-authors [1].

On figure 3 as an example, a window of the program interface is shown. Red dots represent the measured WRC data for the dune sand [2]. In the upper left corner – a set of parameters identified using data on the main branches. Black diamond-shaped dots (connected by a solid curve) represent the results of fit-approximating the main branches (directions indicated by arrows), as well as the results of predicting for the three primary wetting branches.

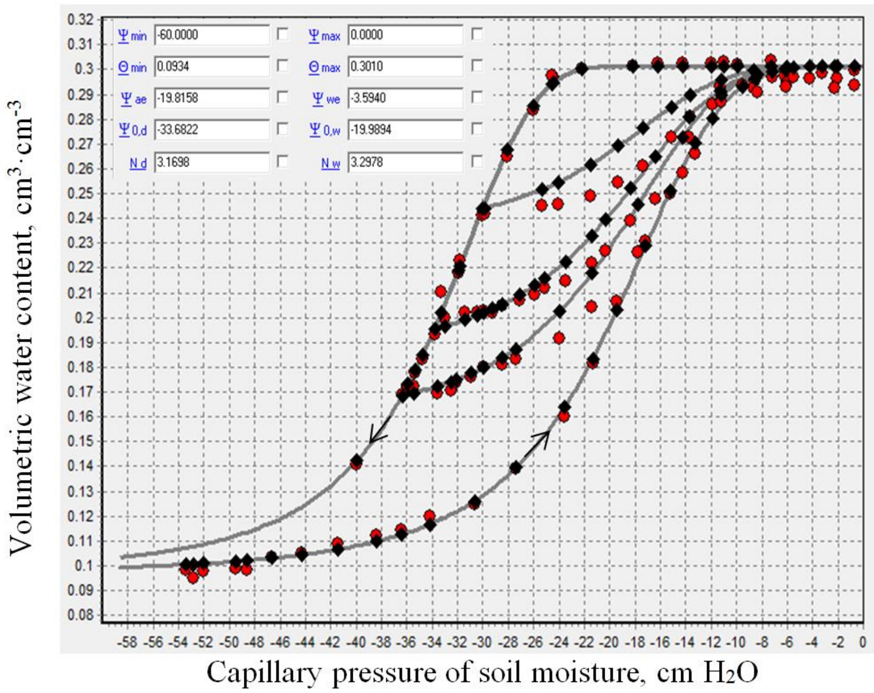


Figure 3. Identification the parameters of the model proposed in this paper by fit-approximating the measured data on the WRC main branches. Predicting for three primary wetting branches of the hysteresis loop of the dune sand [2].

In addition, using the parameters shown on Figure 2, the primary drying branch, the secondary wetting branch and the tertiary drying branch of the white silica sand [1] were predicted. The total results of calculations for this soil are summarized in Table 1. It shows the errors of the four compared models. As errors there were used the average absolute values of the deviations of the calculated results for fit-approximating the MDC and MWC data, predicting the primary drying and wetting branches, the secondary drying and wetting branches, the tertiary drying and wetting branches from the measured WRC data. The minimum errors are indicated in bold.

**Table 2.** Comparison of the four models by the error criterion to the mean absolute value of the deviation of the simulation results from the measured WRC data for the dune sand [2]

| Model | Branches | | |
|---|---|---|---|
| | Main | Primary Wetting | Primary Drying |
| Scott et al. [3] | 0.0027 | 0.0074 | 0.0096 |
| Kool-Parker [4] | 0.0080 | 0.0096 | 0.0151 |
| Huang et al. [1] | 0.0031 | **0.0057** | 0.0096 |
| This paper | **0.0022** | 0.0067 | **0.0094** |

As can be seen from Table 2, with respect to two of the three types of branches of the WRC hysteresis loop, the error of the model proposed by the authors of this paper is lower in comparison with other models.

The concepts that form the basis of the proposed theory, of course, require a more thorough experimental verification. But already here one can argue that they are more reasonable than the published assumption that the branch of the hysteresis loop of the water-retention capacity of the soil, which starts from the last reversal point, intersects with the previous branch at the penultimate reversal point [1]. Of course, a model based on this assumption cannot have an undesirable "artificial pump effect." However, such a model cannot be physically adequate. Indeed, such an assumption means the possibility of crossing any random number of branches corresponding to the same type (sorption or desorption) of equilibrium of soil moisture at the same point. This means that at this point the function $\mu = d\theta/d\psi$ takes an unlimited set of values, which is absurd.

More preferable is the hypothesis supported by the authors, according to which only two values of the function $\mu = d\theta/d\psi$ corresponding to two different (sorption and desorption) types of equilibrium of soil moisture correspond to each point of the hysteresis loop. Such views fully agree with the notions of the nature of the phenomenon of hysteresis of the water-retention capacity of the soil, and in the model constructed on their basis, the undesirable "artificial pump effect" is absent [12] if the values of the model parameters do not go beyond physically justified boundaries. The practical possibility of determining such boundaries is due to the fact that the parameters of the model described in this paper are offered a physical interpretation.

According to the authors, the problem that is typical for most models of the WRC hysteresis is not that these models are characterized by the drift of the values of the volumetric water content within the main branches when the capillary pressure oscillates in a fixed range (this is quite understandable), but this problem consists in the fact that at incorrectly set values of parameters this drift leads to the emergence of values of volumetric water content beyond the main branches. In turn, the problem of incorrect parameter values reduces to the problem of physical interpretation of parameters. If the parameters have no physical meaning, then they cannot be estimated in advance by other physical indicators. In addition, if such parameters are estimated by fit-approximating the main branches, this does not mean that when the result is extrapolated, physically acceptable predictions of the scanning branches will be obtained.

A completely different situation if the model parameters are physically interpreted. In this case: first, they can be estimated from indirect data; Secondly, the use of a physical model with parameters identified by fit-approximating the data on the main branches allows us to reasonably extrapolate the result of fit-approximation and to predict the scanning branches that do not go beyond the main branches of the WRC hysteresis loop.

Thus, the authors believe that the use of models with artificially closed hysteresis loops formed by scanning branches is a poorly promising direction of mathematical modeling. The authors urge that efforts be concentrated on the development of physically based mathematical models. As such an example, the model described in this paper is proposed.

## 4. Conclusion

The mathematical model proposed by the authors of this paper corresponds to physical concepts in relation to the phenomenon of hysteresis of the soil water-retention capacity. Undesirable "artificial pump effect" is not revealed. The application of irrigation norms calculated with the help of this model prevents the percolating the excess moisture under the action of gravity beyond the root layer of the soil, which minimizes the unproductive losses of irrigation water. The use of the proposed model in the development of farming technologies, as well as in substantiating land reclamation measures, will contribute to optimizing the water-air and nutrient regimes of the soil, as well as the rational use of water resources and agrochemicals.

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