The relative hydraulic conductivity model of soil «Guelph Loam»

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Abstract. The relevance of the study is closely related to the urgent demands of society for the development of technologies that allow saving water resources, as well as agrochemicals when cultivating agricultural crops on irrigated lands. The goal outlined by the authors is to fill in the missing ideas about the physical nature of the interactions of the solid and liquid phases of the soil for the development of hydraulic functions, such as its moisture conductivity. The subject of the study is the most important patterns that control the water-physical properties of the soil. The research method is mathematical modelling. The work uses the proposed original function of soil moisture conductivity, which has parameters that allow interpretation. The correlation estimates of the modelling results and experimental data from the literature are given. Two options for setting the exponential parameter of the moisture conductivity function are discussed, including an option that allows eliminating the possible undesirable methodological effect of crossing the scanning and main branches of hysteresis of the water physical properties of the soil. The method has potential for effective application in precision irrigated agriculture.

1 Introduction

The premise of this study is not only the need for predictive assessments of soil moisture dynamics to save irrigation water, but also to prevent unproductive losses of agrochemicals caused by the leakage of agrochemicals from the root zone of the soil [1]. The value of research results is steadily increasing in the context of climate change and a noticeable increase in the frequency of weather anomalies during the growing season. The main obstacle to the development of a method for modeling the hydrophysical properties of soil is the incompleteness of comprehensive knowledge about the physical principles of interaction between the liquid and solid phases of the soil. Awareness of this incompleteness in this area of soil physics gives rise to a scientific problem. The authors of this article are caring out fruitful research in the direction of finding a solution to this problem. The purpose of the

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study is to expand knowledge about the physical principles of the energetic status of soil, taking into account the hysteresis phenomenon. The stated goal is achieved by solving the following tasks [1, 2]:
• theoretical description of the interaction between solid and liquid phases of soil within the framework of classic foundation;
• quantitative description of soil moisture conductivity as a functional dependence on the volumetric soil moisture
• justification of the possibility of using the same values of the exponential parameter to eliminate the undesirable methodological effect, potentially manifested in the intersection of scanning and main branches of the hysteresis of soil water retention;
• assessment of the closeness of the correlation between the modeling results and measurement data from a literary source. [1].

2 Materials and methods

To successfully find a solution to the problems specified in the introduction, a number of original techniques were used:

• theoretical description of the soil hydrophysical properties based on classical physical concepts about the features of the interaction of soil moisture with a solid phase, caused, as is known, by the surface tension of water, as well as the adsorption of water molecules on the surface of soil granules and structural elements;

• description of the soil hydrophysical properties in a hysteresis sweep using parameters that allow physical, statistical and geometric;

• development of software for calculating the soil hydrophysical properties taking into account the hysteresis phenomenon;

• carrying out computational experiments to verify the original mathematical model of the proposed by the authors with the measured data in two versions of setting the exponential parameter [1-4].

As is known, interphase interactions in the soil with the participation of water have a capillary-sorption nature. The capillary component of this interaction is determined by the forces of adhesion of water molecules at the boundary of the abiotic phases of the soil, which are usually called the surface tension of water. The sorption component of the interaction in question is determined by the Van der Waals forces. This property is usually described as the dependence of the volumetric water content in the soil θ [$cm^3 \cdot cm^{-3}$] on the capillary pressure of soil moisture ψ [cm H_2O] and named WRC. By agreement between specialists, it is generally accepted that under a flat surface of the interface between the liquid and gas phases of the soil, the ψ is zero. The dependence of capillary pressure on the curvature of the phase boundary is well described by the well-known Young-Laplace law. Soil WRC is characterized by hysteresis, which manifests itself in the ambiguous nature of the dependence of the volumetric water content of the soil on the capillary pressure of moisture. Differences in the values of θ [$cm^3 \cdot cm^{-3}$] at one value of ψ [cm H_2O]. depend on the history of the moisture state in the soil. If the soil moisture reaches the considered state from a “wetter” state of the soil, then the soil moisture usually exceeds that achieved by moisture from a “drier” state of the soil. The phenomenon of hysteresis is due to the following reasons: firstly, the inconstancy of the area cross-section of the soil transit pores (the "bead effect"); secondly, the presence of dead-end pores in which air can be retained. For the second reason, the capillary pressure of air entering saturated soil at the initial stage of drying, as a rule, does not coincide with the capillary pressure of water entering moistened soil at the final stage of soil saturation with moisture. In accordance with the above, a physically substantiated WRC model has been developed for the first time in a number of papers, among the authors of which are the authors of this original work. In addition, on the basis of this model, a functional description of the relative hydraulic conductivity k/k_s (RHC - the ratio of soil moisture conductivity to the moisture filtration coefficient) has been formulated using the well-known Mualem formula [5].

The developed original (alternative) WRC function and the formulated RHC function of form a system of soil hydraulic functions with a single set of parameters that have physical and statistical meaning. This system of hydraulic functions was subjected to strict comparative analysis using the well-known Van Genuchten system of functions [1-4, 6, 7]. For the objectivity of the results, the comparative analysis used original data from an independent authoritative literary source - the Mualem catalog [8]. Using [1-4, 6, 7], we will remind readers of the original relationships we previously proposed, which formulate the above-mentioned models [9-11]: WRC-VG, original water-retention capacity according to Van Genuchten [9]; RHC-MVG, original relative hydraulic conductivity according to Van Genuchten [9]; WRC-KT, improved Kosugi WRC function [10, 11]; RHC-MKT, improved RHC function according to Kosugi [10, 11]; WRC-HT, alternative (proposed) WRC function [1-4, 6, 7, 12, 13]; RHC-MT, alternative (proposed) function of relative hydraulic conductivity [1-4, 6, 7, 12, 13]:

$$\frac{k}{k_s} = \begin{cases} \sqrt{S_e}\left(1-\left(1-S_e{}^{-1}\right)\exp\left(\frac{8}{n\pi}\right)\right)^{-2}, & \theta_R \le \theta < \theta_S; \\ 1, \ \theta = \theta_S. \end{cases} \quad (1)$$

Let us characterize the quantities included in Eq.1 [9-11]: $S_e = (\theta - \theta_r)/(\theta_s - \theta_r)$ - effective soil moisture saturation, θ_s [$cm^3 \cdot cm^{-3}$] – volumetric water content at saturation; θ_r [$cm^3 \cdot cm^{-3}$] – volumetric (residual) water content; parameter n ($n > 1$) of Van Genuchten functions [6] is empirical and have no physical meaning; The parameter n in the improved and alternative functions allows physical-statistical integration (n characterizes the pore size distribution).

The authors then examine the applicability of the function presented in Eq.1 to describe the RHC of the soil using independent data. The Mualem catalogue [8] contains an object for which both the WRC hysteresis and the RHC data are presented: this is the soil «3407 Guelph Loam». A careful analysis of the literature revealed that publications devoted to modelling the WRC hysteresis of the soil most often cite the developments of Scote [14], as well as Kool and Parker [15]. It is interesting to note that the Kool and Parker model [15] uses the scanning branch calculation algorithm proposed by Scott et al. [14]. In this case, the model of Scott et al. uses the WRC-HT_0 proposed by Haverkamp et al. [16], and the model of Kool and Parker uses the WRC-VG proposed by Van Genuchten [9]. For convenience, we will further denote the hysteresis models being compared using the abbreviations introduced by us in previous works: Hys-KPVG - Kool and Parker hysteresis model with Van Genuchten water retention [1-4, 6, 7, 12, 13]; Hys-SKT - hysteresis model with the improved Kosugi water retention [1-4, 6, 7, 12, 13]; Hys-SHT - hysteresis model with the alternative (suggested) water retention [1-4, 6, 7, 12, 13]; Hys-SKT_0 - hysteresis model with the original Kosugi WRC function [1-4, 6, 7, 12, 13]; Hys-SHT_0 - hysteresis model proposed by Scott et al. with the original Haverkamp et al. WRC function [1-4, 6, 7, 12, 13].

It should be noted that the algorithm for calculating the scanning branches of the WRC hysteresis of the soil proposed by Scott et al. [14] is not without a drawback. This drawback is undesirable methodological effect; it is called the «pump effect». To eliminate this effect, it is possible to propose using the same values of the exponential parameter for both the drying and moistening branches ($n_d = n_w$). Of course, if we accept this assumption, then we should expect a decrease in the accuracy of the assessment of the scanning branches of the WRC hysteresis of the soil. However, this decrease may well turn out to be insignificant in a statistical sense. At the same time, when accepting the condition $n_d = n_w$, we exclude the possibility of taking into account the RHC hysteresis as a function of θ. To do this, we must again refer to Eq.1. And then a very important question arises: does the phenomenon of hysteresis take place for the property of soil to conduct moisture, described by the dependence, the argument of which is θ? For the studied soil in the catalog of Mualem it is noted that the phenomenon of hysteresis in this case is not observed. In other words, the absence of the phenomenon of hysteresis of RHC as a function of θ, confirmed by the measured data for the studied soil, proves the admissibility of accepting the condition $n_d = n_w$, which, in turn, favors the elimination of the undesirable methodological «pump effect» in calculating the scanning branches of the WRC. In order to finally confirm the idea that what was revealed for the studied soil is characteristic of all soils, further research is necessary. Nevertheless, in relation to the studied soil, we can already state on the basis of the available measured data that the phenomenon of hysteresis is not characteristic of RHC as the function of θ, while this phenomenon manifests itself quite noticeably for WRC. We should also note that if we consider hydraulic conductivity as a function of capillary pressure, a hysteresis loop will be visible. However, it should be understood that this loop will be methodically induced by the hysteresis of the WRC.

Next, we will move on to computational experiments that will allow us to draw conclusions about the effectiveness of a particular hydraulic function in relation to the approximation of measured data on the WRC, as well as in relation to the predictive assessment of the values of the function of RHC of the studied soil «3407 Guelph Loam» from the Mualem catalog [8]. To carry out these experiments, we will use two computer program packages «SoilHysteresis-V.1.0» [17] and «SoilHydrophysics-V.1.0» [18], in the development of which some of the authors of this publication took part.

3 Results and discussions

The parameters of the soil hydraulic function in Eq.1 were taken from [2]. The parameter values were identified by the point approximation method of the measured data on the main (boundary) branches of the hysteresis of the WRC of the studied soil «3407 Guelph Loam» using the computer program «SoilHysteresis-v.1.0» [17] for two variants of the computational experiment: $n_d \neq n_w$ и $n_d = n_w$ [2] (indexes «*d*» (*drying*) and «*w*» (*wetting*) used respectively for drying and wetting branches of the hysteresis loop, the index «*e*» (*entrance*) is used). Data from [2] illustrates the closeness of the correlation between the modelling results and the measured data on the main (boundary) branches of the WRC hysteresis loop of studied soil. From [2] it is evident that in the variant $n_d = n_w$ there is some increase in the errors of parametric identification of hydraulic functions to the variant $n_d \neq n_w$ according to λ-criterion [19]. We understand that under the condition $n_d = n_w$ the undesirable methodological «pump effect» is eliminated. But at what price is this elimination achieved? From the comparison of the two variants of the computational experiment we see that the error of parametric identification increases significantly in the variant $n_d = n_w$ compared to the variant $n_d \neq n_w$ only for two of the five models: Hys-SKT and Hys-SKT_0 [2]. However, in the opinion of the authors of this article, the importance of eliminating the possible undesirable methodological «pump effect» outweighs the potential costs that may arise in estimating the values of hydraulic functions when using the same values of the exponential parameter in these functions. From [1, 2] it is clear that for the$n_d \neq n_w$ variant the parametric identification error is significantly reduced when the functions contain the additive parameter, which takes into account the difference between the «air entry pressure» and the «water entry pressure». Due to the lack of measured data in the range of positive values of the capillary pressure of soil moisture, the additive parameter takes positive values close to zero for the wetting branch (see Figs. 1a and 1b). At the same time, for the drying branch, the parameter takes slightly negative values in full agreement with the available measured data. This soil is not entirely typical in the sense that the main branches of drying and wetting of the hysteresis loop converge at a point close to the zero value of the capillary pressure of moisture. Therefore, for the $n_d = n_w$ variant, in which the sensitivity of the models to variations in the parameter values is somewhat reduced, the use of the additive parameter does not significantly affect the errors of parametric identification of the hydraulic functions. Nevertheless, we repeat that this example is not typical, and for other soils one should expect a significant reduction in the errors of parametric identification when using the additive parameter.

Figures $1a$ and $1b$ illustrate the results of a computer experiment (variant $n_d = n_w$) on the parametric identification of hydraulic functions, which are used in the Hys-SKT and Hys-SHT hysteresis models, using the point approximation method of measured WRC data on the main (boundary) branches of drying and wetting of the soil under study [2]. The obtained results indicate the advantages of the WRC-KT and WRC-HT functions over the other hydraulic functions from [2]. However, it is worth noting that the WRC-HT and RHC-MT pair has a simpler and more convenient in practical terms description in the class of elementary functions in contrast to the WRC-KT and RHC-MKT pair. Therefore, in further calculations, the authors give preference to the WRC-HT and RHC-MT pair of hydraulic functions. Fig. 2 illustrates the assessment of the relative hydraulic conductivity using the RHC-MT function and the parameters of the WRC-HT function identified from the data of direct measurements of the main branches of the WRC hysteresis of the studied soil (the «SoilHydrophysics-V.1.0» software package was used [18], in the development of which some of the authors of this publication took part). The correlation coefficient R = 0.98267 is statistically significant with a confidence level of 0.99.

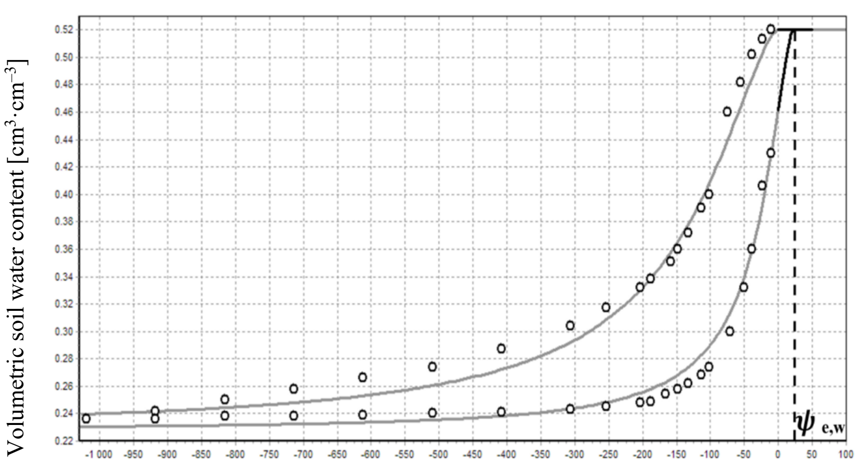

Fig.1 ***a.*** Results of point approximation of WRC-data on the main (boundary) branches for the «3407 Guelph loam» soil using the model Hys-SHT ($n_d = n_w$).

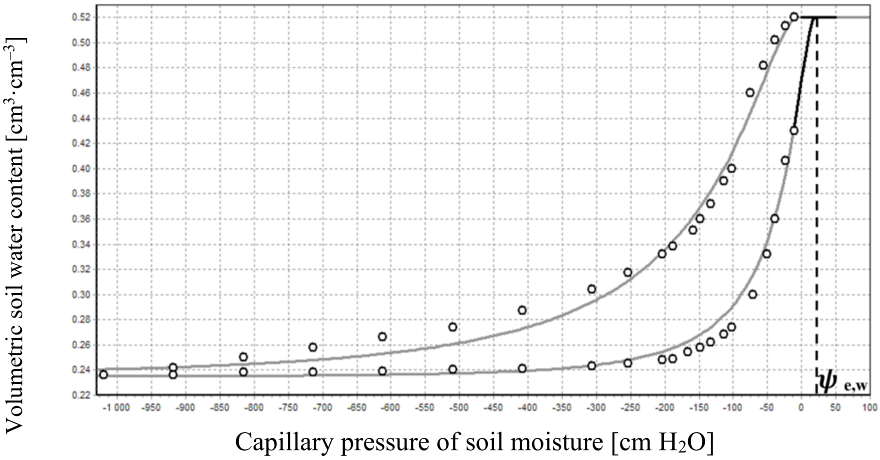

Fig.1 *b*. Results of point approximation of WRC-data on the main (boundary) branches for the «3407 Guelph loam» soil using the model Hys-SKT ($n_d = n_w$).

It is evident from Fig. 2 that the error in the prognostic assessment of the relative hydraulic conductivity using the RHC-MT and WRC-HT based on the direct WRC measurements of the main branches of drying and wetting [2] of the studied soil is very small. We would like to draw the reader's attention to the fact that this result was obtained in a computational experiment on the parametric identification of the RHC-MT and WRC-HT hydraulic functions in the $n_d = n_w$ variant. This means that the phenomenon of RHC hysteresis as a function of θ does not really manifest itself for the studied soil. This circumstance allows us to reasonably eliminate the undesirable methodological «pump effect» when modelling the WRC hysteresis of the studied soil. But will such an approach be valid for other soils?

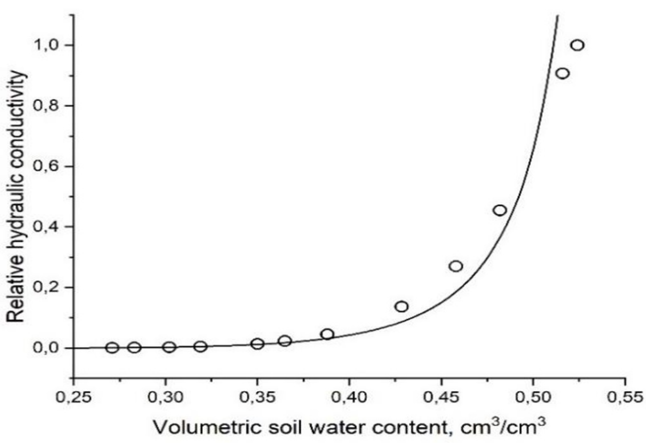

Fig.2. Results of estimating the relative hydraulic conductivity using the proposed RHC-MT function and the parameters of the WRC-HT function identified from direct measurements of the main branches of the WRC\hysteresis of the studied soil [2]: points are experimental data; the solid curve is the result of modelling in the computational experiment $n_d = n_w$.

If hydraulic conductivity is considered as a function of ψ, which characterizes the capillary-sorption interaction of the liquid and solid phases of the soil, then such a function should include parameters that take into account such a phenomenon as hysteresis. If hydraulic conductivity is considered as a function of θ, then only the structure of the pore space of the soil is taken into account, and the θ characterizes the proportion of filling this space with water. It is this proportion of filling the soil pores with the liquid phase that will determine the ability of the soil to conduct water. Consequently, at different values of ψ corresponding to the same θ, the hydraulic conductivity will be the same. Therefore, if the argument of the RHC function is ψ, then this function is hysteretic. If the argument of this function is θ, then the function is not hysteretic. Now let us turn to the RHC-MT hydraulic function from [2]. It contains the exponential parameter n. In the theoretical justification and mathematical formulation of the RHC-MT and WRC-HT functions, this parameter was given the meaning of a value inversely proportional to the standard deviation - the parameter of pore size distribution. In such a physical-statistical interpretation, the drying branch and the wetting branch of the WRC hysteresis are considered conditionally as the same-named branches of soils with different pore distributions. That is, the wetting branch, which is located below the drying branch, corresponds to a higher value of the exponential parameter compared to the drying branch. This means that the wetting branch corresponds to a more uniform pore structure (the dispersion of pore sizes of such soil is lower) compared to the drying branch. In other words, the wetting branch corresponds to soil in which there are more small pores of the same size compared to the drying branch. In this case, for the wetting branch due to internal friction (rheological properties) of the liquid phase, one should expect lower values of the relative hydraulic conductivity of the soil compared to the drying branch, which is fully consistent with the formulas in [2]. If this phenomenon is not observed in the experiment with the studied soil, then the factor of internal friction of the liquid phase is not significant for this soil. The following question arises: what factor can we take into account the efficiency threshold of the internal friction factor of soil moisture? In our opinion, this parameter is the volumetric residual soil moisture θ_r. Consequently, if we consider soils for which the rheological properties of the liquid phase remain unchanged in the range from θ_r to θ_s, then the hydraulic conductivity of such soils as a function of θ is not hysteretic. Obviously, the soil studied in this work also belongs to such soils. In other cases, the phenomenon of hysteresis should be expected. Hence, the importance of accurately determining the parameter θ_r. is evident. If this parameter is set correctly, it is possible to justifiably refuse to take into account the RHC hysteresis, when RHC is a function of θ, and also to eliminate the undesirable «pump effect» by using $n_d = n_w$ from [2] for the drying and wetting branches of the WRC hysteresis of the soil.

4 Conclusions

The relevance of this study is determined by the need for the original results obtained here on modeling the hydraulic conductivity of the soil, necessary for predictive calculation of the dynamics of soil moisture and the development of management effects on the agroecosystem in the conditions of irrigated agriculture. The issues considered deepen the theory of soil hydrophysics in relation to such soil properties as water retention and hydraulic conductivity. Of particular theoretical interest are the results on accounting for the hysteresis phenomenon. The applied significance of the results obtained in the work lies in the possibility of predicting the moisture reserves of the root layer of the soil [13]. The value of the original results obtained in this work increases significantly in the context of climate change and an increase in the frequency of weather anomalies accompanying these changes during the growing season. In this paper, an attempt was made to overcome conceptual and methodological

barriers to developing an approach to modelling the hydrophysical properties of soils [10, 13]:
• substantiated consideration of the energetics of the state of soil moisture in the hysteresis sweep based on classical theoretical concepts about the nature of the studied soil properties;
• formulation of the relationship describing the RHC as a functional dependence on the volumetric water content;
• substantiation of the requirements, upon fulfillment of which: firstly, the undesirable methodological «pump effect» is excluded, and also upon fulfillment of which the RHC as a function of the volumetric water content is not hysteresis;
• estimated calculations of the values of hydraulic functions were carried out in comparison with experimental data in two variants of the computational experiment (with different and equal values of the exponential parameter) [2, 13];
• fundamental issues of the possibility and necessity of taking into account the hysteresis of the hydraulic conductivity of the soil were discussed.

The use of suggested mathematical models of hysteresis allows minimizes the risk of contamination of groundwater and open water bodies with chemicals [20-26].

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