Research Article

Modeling of Hydrophysical Properties of the Soil as Capillary-Porous Media and Improvement of Mualem-Van Genuchten Method as a Part of Foundation Arrangement Research

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Within the concepts about the capillarity and the lognormal distribution of effective pore radii, a theoretical justification for function of differential water capacity and its antiderivative (function of water-retention capacity in form of a dependence of the soil volumetric water content on capillary pressure of the soil moisture) is presented. Using these functions, the ratio of soil hydraulic conductivity function to the filter coefficient is calculated. Approximations to functions describing the water-retention capacity and relative hydraulic conductivity of the soil have been suggested. Parameters of these functions have been interpreted and estimated with applying the physical and statistical indices of the soil.

1. Introduction

In laboratories usually do not measure the differential water capacity (DWC) function $\mu = \mu(\psi)$ but its antiderivative-water sorption equilibrium isotherm as a dependence of the volumetric soil moisture θ ($\text{cm}^3 \cdot \text{cm}^{-3}$) on capillary pressure of the soil moisture ψ ($\text{cm H}_2\text{O}$). The dependence $\theta(\psi)$ is an indicator of water-retention capacity (WRC) of soil. Calculating the values of DWC is usually limited to interpolating the measured WRC data and to selection of the approximating function, which is then used in the computation by the formula $\mu = d\theta/d\psi$. However, differentiation of approximations is by definition an unstable operation, which can lead to physically absurd results. As a negative example, the degree function was previously widely used for the interpolation of modified WRC points for the subsequent calculation of

the DWC values. However, there are some positive examples of the use of WRC approximations, which include the model:

$$S_e = \begin{cases} (1 + (-\alpha\psi)^n)^{-m}, & \psi < 0; \\ 1, & \psi \geq 0, \end{cases} \quad (1)$$

where $S_e = (\theta - \theta_R)/(\theta_S - \theta_R)$ is the relative volumetric water content (effective saturation); θ_S is the volumetric water content under conditions of moisture-saturated soil ($\text{cm}^3 \cdot \text{cm}^{-3}$); θ_R is the volumetric water content, which corresponds to the minimum of specific volume of water as liquid in soil ($\text{cm}^3 \cdot \text{cm}^{-3}$); α ($\text{cm H}_2\text{O}^{-1}$), n , and m are parameters.

When $m = 1 - 1/n$, model (1) is the WRC proposed by Van Genuchten [1]. When $m = 1$, relation (1) has the form of the precursor's WRC [2–4]. Van Genuchten uses model (1) to

calculate the ratio of the soil hydraulic conductivity function (HCF) $k = k(\psi)$ to filter coefficients of soil moisture k_s by Mualem method [5]:

$$\frac{k}{k_s} = \sqrt{S_e} \left(\frac{\int_0^{S_e} (dz/\psi(z))}{\int_0^1 (dz/\psi(z))} \right)^2. \quad (2)$$

Description of hydrophysical properties of the soil using WRC (1) and HCF (4), having common parameters, is called Mualem-Van Genuchten method.

The purpose of this paper is as follows:

- (i) theoretical justification and formation of a system of functions with common and adequately interpreted parameters, which combine DWC, its primitive in WRC form, and the ratio of HCF to the filter coefficient of soil moisture;
- (ii) approximation of $\theta(\psi)$ and $k(\psi)/k_s$ in the class of elementary functions and parameter estimation of approximating functions by the physical parameters of the soil.

2. Materials and Methods

2.1. Differential Water Capacity and Water-Retention Capacity of the Soil. It is known that pores in natural structured soils are preferably capillary. In cross section capillaries are very different by the configuration and area, which is caused by the random combination of contacting soil particles of varying shape and size. As a basis for hydrophysical properties of the soil modeling view of the system of cylindrical pores of circular cross section is adopted. This system is equivalent to the actual pore space of the soil by its capillary properties. The model of random lognormal value—the effective radius of the pores—is used to describe the distribution of the volumes of soil capillary [6–9]. By analogy with Kosugi work, $\bar{r} = (r - r_{\min})/(r_{\max} - r)$ is accepted as an effective radius of the pores of the soil, where r is radius of the pore; $r_{\min}$ is radius of the smallest pore; $r_{\max}$ is radius of the widest pore [10]. The relations for calculating the proportion of pore volume Θ are recorded, taking into account the random nature of the cross section of soil pores. This proportion accounted for the capillaries, starting with the smallest and ending with effective pore radius $\bar{r}$:

$$\frac{d\Theta(\bar{r})}{d\bar{r}} = f(\bar{r}) = \frac{\exp(-\ln^2(\bar{r}/\bar{r}_0)/(2\sigma^2))}{\bar{r}\sigma\sqrt{2\pi}}, \quad (5)$$

$$\Theta(\bar{r}) = \int_0^{\bar{r}} f(\bar{r}) d\bar{r},$$

Using the variable $y = z^{1/m} = (1 + (-\alpha\psi)^n)^{-1}$, (2) reduces to

$$\frac{k}{k_s} = \sqrt{S_e} \left(\frac{\int_0^{S_e^{1/m}} y^{m-1+1/n} (1-y)^{-1/n} dy}{\int_0^1 y^{m-1+1/n} (1-y)^{-1/n} dy} \right)^2. \quad (3)$$

In the case $m = 1 - 1/n$, (3) permits a simple analytical calculation, and the result of integration is as follows:

$$\frac{k}{k_s} = \begin{cases} \sqrt{S_e} (1 - (1 - S_e^{1/m})^m)^2 = (1 + (-\alpha\psi)^n)^{-m/2} (1 - (1 - (1 + (-\alpha\psi)^n)^{-1})^m)^2, & \psi < 0; \\ 1, & \psi \geq 0. \end{cases} \quad (4)$$

where $f(\bar{r})$ is lognormal distribution density of the random variable $\bar{r}$; $\ln \bar{r}_0$ and σ are the most probable value and standard deviation of the logarithms of the effective soil pores radii, respectively. The variable $x = \ln(\bar{r}/\bar{r}_0)/(\sigma\sqrt{2})$ is introduced and formula (5) is rewritten in the way

$$\frac{d\Theta}{dx} = \frac{\exp(-x^2)}{\sqrt{\pi}}, \quad (6)$$

$$\Theta = \int_{-\infty}^x \frac{\exp(-x^2)}{\sqrt{\pi}} dx = \frac{\operatorname{erf}(x) + 1}{2} = \frac{\operatorname{erfc}(-x)}{2},$$

where $\operatorname{erf}(x)$ is error function ($\operatorname{erf}(x_0) = 0$ and $\Theta(x_0) = 1/2$, when $x = x_0 = 0$); $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$.

From formulas (6) the relation should be:

$$4(1 - \Theta(x))\Theta(x) = 1 - \operatorname{erf}^2(x). \quad (7)$$

The approximation by Winitzki [11] was used $1 - \operatorname{erf}^2(x) \approx \exp(-x^2(4/\pi + ax^2)/(1 + ax^2))$, $a = 8(\pi - 3)/(3\pi(4 - \pi))$. We reduced it to a simpler form: $1 - \operatorname{erf}^2(x) \approx \exp(-x^2)$. The approximate equality follows from formulas (6) and (7): $d\Theta/(\Theta(1 - \Theta)) \approx (4/\sqrt{\pi})dx$; it obtains an analogue of the Verhulst equation. Decision of the resulting nonlinear ordinary differential equation of the first order with the boundary condition $\Theta(x_0) = \Theta_0 = 1/2$ is logistic curve, which is approximately the ratio $\Theta = \Theta(x)$ in a class of elementary functions:

$$\Theta(x) = \frac{\operatorname{erfc}(-x)}{2} \approx \frac{1}{\exp(-4x/\sqrt{\pi}) + 1}. \quad (8)$$

Given the connection between the values of x and $\bar{r}$, reduce formula (8) in the form

$$\Theta(\bar{r}) = \frac{1}{2} \operatorname{erfc}\left(-\frac{\ln(\bar{r}/\bar{r}_0)}{\sigma\sqrt{2}}\right) \approx \frac{1}{1 + (\bar{r}/\bar{r}_0)^{-4/(\sigma\sqrt{2\pi})}}. \quad (9)$$

The possibility of moving from $\bar{r}$ to ψ and from Θ to S_e is considered for conversion of formula (9). The difference between the absolute pressures under the curved boundary between “air-capillary moisture” P and a flat free water

surface P_a is called a capillary moisture pressure, which is calculated by the law of Laplace: $\psi = P - P_a = -\beta/r$, where r is soil capillary radius; $\beta = (2\gamma \cos \phi)/(g\rho_w)$; γ is the surface tension coefficient of soil moisture at the interface with the air; ϕ is contact angle of the surface of soil particles with water; g is acceleration of gravity; ρ_w is density of water. Under the physical modelling of soil drainage using a pneumatic press, water displacement is achieved by exposure of the excess pressure of atmospheric gases. Dissolution of the air in water occurs with the increase of gas pressure above the water in the pores of the soil, from the normal external atmospheric pressure P_a to the value P_{ae} . Excess gas pressure is transferred to the water; the absolute pressure is also increased. When excess gas pressure reaches a value $\Delta P_{ae} = P_{ae} - P_a$, strength of the interaction between water molecules and the surface of soil particles weakens so that the water goes into the category of free gravitational water which follows from the soil through the membrane into a tray; the air occupies the vacant pore volume. Excess gas pressure in the pneumatic press with respect to the external atmospheric pressure corresponds to the value of the capillary pressure of moisture in the soil of the largest pore $\psi_{ae} = -\Delta P_{ae} = -\beta/r_{\max} < 0$. This value is called “bubbling

pressure”; it will be considered as the “initial point” of the capillary pressure. With use of $\bar{r} = (r - r_{\min})/(r_{\max} - r)$, for case $r_{\min} \ll r$ (accept $r_{\min} = 0$) the formula is derived:

$$\begin{aligned}\psi - \psi_{ae} &= -\frac{\beta}{r_{\max}\bar{r}}; \\ \psi_0 - \psi_{ae} &= -\frac{\beta}{r_{\max}\bar{r}_0},\end{aligned}\quad (10)$$

where $\bar{r}_0 = r_0/(r_{\max} - r_0)$; r_0 is the radius of the soil pore, which corresponds to the most probable value of $\ln \bar{r}_0$ of the random variable $\ln \bar{r}$.

Applying formulas (10), enter the following values:

$$\begin{aligned}\alpha &= -\frac{1}{\psi_0 - \psi_{ae}} = \frac{r_{\max}\bar{r}_0}{\beta}; \\ n &= \frac{4}{\sigma\sqrt{2\pi}}.\end{aligned}\quad (11)$$

Using law of Laplace and formula (11), relationship (9) can be represented as

$$\Theta = \begin{cases} \frac{1}{2} \operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right) \approx \frac{1}{1 + (-\alpha(\psi - \psi_{ae}))^n}, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}. \end{cases}\quad (12)$$

Moistening of the soil begins with water filling the smallest pores, and only after they are saturated with moisture, does water start to occupy the larger pores. Drainage of the soil begins with air displacing the water from the largest pores, and only after they are emptied, does air start to occupy the smallest pores. The capillary pressure is the same at all points of topologically closed water space (law of Pascale). The biggest radius among all the moisture-filled pores determines the pressure. These factors make it possible to identify the proportion of the pores volume of Θ with an effective radius not more than $\bar{r}$ with the value of the relative volumetric water content (effective saturation) $S_e = (\theta - \theta_R)/(\theta_S - \theta_R)$ at the capillary pressure ψ , which uniquely corresponds to $\bar{r}$. So, mathematical identity $\Theta \equiv S_e$ is physically reasonable.

Relation $S_e = S_e(\psi)$ is a WRC by the definition, so it allows transferring relation (12) to the following form:

$$\begin{aligned}S_e &= \begin{cases} \frac{1}{2} \operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right), & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}. \end{cases}\end{aligned}\quad (13a)$$

$$S_e \approx \begin{cases} \frac{1}{1 + (-\alpha(\psi - \psi_{ae}))^n}, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}. \end{cases}\quad (13b)$$

Relation $\theta = \theta(\psi)$ is an antiderivative with respect to the relative DWC function $\mu = \mu(\psi)$:

$$\mu = \begin{cases} -\frac{n(\theta_S - \theta_R)}{4(\psi - \psi_{ae})} \exp\left(-\pi\left(\frac{n}{4}\right)^2 \ln^2(-\alpha(\psi - \psi_{ae}))\right), & \psi < \psi_{ae}; \\ 0, & \psi \geq \psi_{ae}. \end{cases}\quad (14)$$

In case $r_{\max} \gg r$ take $\psi_{ae} = 0$, and from formulas (13a) and (14) we arrive at the relations, previously obtained by Kosugi [10].

2.2. The Ratio of Hydraulic Conductivity Function to Filter Coefficients of Soil Moisture. Here are not any empirical

relationships for application in the calculation by Mualem method, which interpolates the measured WRC data, by analogy with Kosugi [10]. Instead of this, the relative DWC function is used. Moreover, this function is theoretically justified in the frames of some concepts about capillarity and geometry of pore space of the soil. According to formulas (13a) and

(13b), the value S_e under the capillary pressure ψ_{ae} reaches 1. So, using the identity $\Theta \equiv S_e$, formula (2) transforms into

$$\begin{aligned} \frac{k}{k_s} &= \sqrt{S_e} \left(\frac{\int_0^{S_e} (dz/\psi(z))}{\int_0^1 (dz/\psi(z))} \right)^2 \\ &= \sqrt{S_e} \left(\frac{\int_{-\infty}^{\psi} (dS_e/d\psi) (d\psi/\psi)}{\int_{-\infty}^{\psi_{ae}} (dS_e/d\psi) (d\psi/\psi)} \right)^2 \\ &= \sqrt{S_e} \left(\frac{\int_{-\infty}^{\psi-\psi_{ae}} (dS_e/d(\psi-\psi_{ae})) (d(\psi-\psi_{ae})/(\psi-\psi_{ae}))}{\int_{-\infty}^0 (dS_e/d(\psi-\psi_{ae})) (d(\psi-\psi_{ae})/(\psi-\psi_{ae}))} \right)^2 \end{aligned}$$

$$\begin{aligned} &= \sqrt{\Theta} \left(\frac{\int_0^{\bar{r}} \bar{r} (d\Theta/d\bar{r}) d\bar{r}}{\int_0^{\infty} \bar{r} (d\Theta/d\bar{r}) d\bar{r}} \right)^2 \\ &= \sqrt{\Theta} \left(\frac{\int_{-\infty}^x \exp(-x^2 + x\sigma\sqrt{2}) dx}{\int_{-\infty}^{\infty} \exp(-x^2 + x\sigma\sqrt{2}) dx} \right)^2 \\ &= \frac{\sqrt{\Theta}}{4} \left(\operatorname{erf}\left(x - \frac{\sigma}{\sqrt{2}}\right) + 1 \right)^2 = \sqrt{\Theta(x)} \left(\Theta\left(x - \frac{\sigma}{\sqrt{2}}\right) \right)^2. \end{aligned} \quad (15)$$

Using the transition from x to ψ , the final formula, which describes the ratio of HCF to filter coefficient of soil moisture, as well as an approximation of this ratio, has been obtained:

$$\frac{k}{k_s} = \begin{cases} \frac{1}{4\sqrt{2}} \sqrt{\operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right)} \left(\operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right) + \frac{2}{n\sqrt{\pi}} \right)^2, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}, \end{cases} \quad (16a)$$

$$\frac{k}{k_s} \approx \begin{cases} \frac{1}{\sqrt{1 + (-\alpha(\psi - \psi_{ae}))^n (1 + \exp(8/(n\pi)) (-\alpha(\psi - \psi_{ae}))^n)}}, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae}. \end{cases} \quad (16b)$$

In the particular case ($\psi_{ae} = 0$), the ratio (16a) leads to the Kosugi formula [10]. Models (13a), (14), and (16a) form a parameter-closed system of soil and hydrophysical functions. Relation of (13b) and (16b) approximates WRC and the $k(\psi)/k_s$ values, relatively, in a class of elementary functions.

2.3. Interpretation of Parameters of the Soil Hydrophysical Functions. Theoretically justified models (13a), (14), and (16a) have the common parameters, for which physical and statistical interpretation is proposed. Parameter $\alpha = r_{\max}\bar{r}_0/\beta$ is determined: (1) by multiplication of the widest pore radius $r_{\max}$ and the effective pore radius $\bar{r}_0$, in which the random variable $\ln \bar{r}$ reaches the most probable value; (2) by β coefficient in formula of Laplace, which describes the capillary properties of the soil. If $r_{\max} \gg r_0$, then $\alpha = r_0/\beta$. Parameter $n = 4/(\sigma\sqrt{2\pi})$ is a value, inversely proportional to σ —the standard deviation of the logarithms of the effective pore radii. Parameter ψ_{ae} is the bubbling pressure on the drainage isotherm of the soil, initially saturated with moisture. Coupling of the parameters α and n with the certain DWC value can be revealed from the relation $\mu_0 = \alpha n(\theta_S - \theta_R)/4$, where μ_0 is the value of $\mu(\psi)$ function calculated using formula (14) with $\psi = \psi_0$, where ψ_0 is capillary pressure that corresponds to the effective pore radius $\bar{r}_0$ (at $\psi = \psi_0$ the effective saturation $S_e(\psi_0) = 1/2$). The DWC function reaches its maximum at the inflection point of WRC curve. Authors consider that it corresponds to the maximum capillary-sorption moisture capacity of the soil [12, 13].

3. Results and Discussion

The measured WRC data are usually used to design the curves with respect to formulas (1) and (4). Here we made simulation of $\theta(\psi)$ dependence applying the data, for which calculating the statistics of lognormal distributed effective soil pore radii $\ln \bar{r}_0 = -1.1087$ and $\sigma = 0.6383$ was given, as well as some characteristics of the capillary properties of the soil pore space $r_{\max} = 0.149 \cdot 10^{-2}$ cm; $\psi_{ae} = -100$ cm H₂O and $\beta = 0.149$ cm² [2, 8, 14, 15] were given. Using formulas (11) and given indices, the parameters of DWC function $\alpha = 0.33 \cdot 10^{-2}$ cm H₂O⁻¹ and $n = 2.5$ were calculated. Then by formula (13a) with usage of α , n , and ψ_{ae} parameters the curve (white circles on Figure 1), which simulates $\theta(\psi)$ data, was depicted. With that, according to formula (16a), the curve (black circles on Figure 1), which simulates the $k(\psi)/k_s$ ratio, was depicted. Formulas (13b) and (16b) have been used to depict curves (1) and (2) (see Figure 1), which represent the approximation to WRC and relative HCF.

The results of the comparative analysis with respect to the proposed models and well-known formulas of Mualem-Van Genuchten are represented gradually in Table 1. The following benefits of the offered soil hydrophysical functions over functions (1) and (4) are revealed. Firstly, taking into account that both systems are closed in the parameters, these parameters are adequately interpreted only in the models proposed here. Secondly, here the methodologically more preferred method for calculating the ratio $k(\psi)/k_s$ is used, which uses the physically justified theory of the soil differential water capacity and does not apply the hardly

TABLE 1: Two systems of soil hydrophysical functions.

Mualem-Van Genuchten system	System proposed in this paper
<p>Approximation to WRC function that interpolates the experimental data</p> $S_e = \begin{cases} \left(1 + (-\alpha\psi)^n\right)^{-m}, & \psi < 0; \\ 1, & \psi \geq 0 \end{cases}$	<p>Water-retention capacity</p> <p>The antiderivative of theoretically justified function of differential moisture capacity and approximation to this antiderivative</p> $S_e = \begin{cases} \frac{1}{2} \operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right) \approx \frac{1}{\left(1 + (-\alpha(\psi - \psi_{ae}))^n\right)}, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae} \end{cases}$
<p>The derivative of the approximation to WRC function</p> $\frac{dS_e}{d\psi} = \begin{cases} m\alpha^n (-\psi)^{n-1} \left(1 + (-\alpha\psi)^n\right)^{-(m+1)}, & \psi < 0; \\ 0, & \psi \geq 0 \end{cases}$	<p>Differential water capacity</p> <p>The function, which is reasonable in terms of the concept of capillarity and lognormal distribution of effective pore radii</p> $\frac{dS_e}{d\psi} = \begin{cases} -\frac{n}{4(\psi - \psi_{ae})} \exp\left(-\pi\left(\frac{n}{4}\right)^2 \ln^2(-\alpha(\psi - \psi_{ae}))\right), & \psi < \psi_{ae}; \\ 0, & \psi \geq \psi_{ae} \end{cases}$
<p>WRC approximation is used with a ratio $m = 1 - 1/n$</p> $\frac{k}{k_s} = \begin{cases} \left(1 + (-\alpha\psi)^n\right)^{-m/2} \left(1 - \left(1 + (-\alpha\psi)^n\right)^{-1}\right)^m, & \psi < 0; \\ 1, & \psi \geq 0 \end{cases}$	<p>The ratio of hydraulic conductivity of soil to the filter coefficients of moisture</p> <p>Theoretically justified function of differential water capacity is used</p> $\frac{k}{k_s} = \begin{cases} \frac{1}{4\sqrt{2}} \sqrt{\operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae}))\right)} \left(\operatorname{erfc}\left(\frac{n\sqrt{\pi}}{4} \ln(-\alpha(\psi - \psi_{ae})) + \frac{2}{n\sqrt{\pi}}\right)\right)^2, & \psi < \psi_{ae}; \\ 1, & \psi \geq \psi_{ae} \end{cases}$
<p>Empirical parameters α and n are estimated by interpolation of WRC data or using some pedotransfer functions</p>	<p>The parameters of soil hydrophysical functions</p> <p>Physical and statistical interpreted parameters α and n are theoretically justified. Estimation the parameters can be made using the indicators of soil:</p> $\alpha = \frac{r_{\max} \bar{r}_0 g \rho_w}{2\gamma \cos \phi} \approx \frac{r_0 g \rho_w}{\sigma \sqrt{2\pi}}; \quad n = \frac{4}{2\gamma \cos \phi}$

FIGURE 1: Comparison of the proposed approximation to the functions of water-retention capacity and hydraulic conductivity of the soil with the simulation data (explanation in the text).

accessible WRC measurements, interpolated by function (1) with the problematic relation $m = 1 - 1/n$. Thirdly, the parameters of models (13a), (13b), (14), and (15) can be estimated using the soil physical and statistical indices.

4. Summary

The theoretical justification for function of the differential water capacity and antiderivative of this function in the form of WRC model are proposed. Mualem-Van Genuchten functions were improved: model (1) with the problematic relation $m = 1 - 1/n$ is not used in calculating the ratio of hydraulic conductivity function to filter coefficients of soil moisture. Theoretically justified function of the differential water capacity is used. The parameters α , n , and ψ_{ae} of soil hydrophysical functions are adequately interpreted within the concept of soil as capillary-porous media. Sufficiently accurate approximations in class of the elementary functions are proposed for WRC and the relative HCF (see Figure 1). The parameters of these approximations are estimated using the statistics of lognormal distribution of the effective radii of pores and capillary indicators of the soil. The system of hydrophysical functions, which are proposed here, makes it possible to improve the accuracy of calculating the dynamics of soil moisture [16] and evaluation of irrigation rates [17], as well as predictions of crop yields [18–22]. These data are particularly important for planning the complicated foundations on weak soils [23], at the predesign-research part of the foundation arrangement researches. Such researches must be held before the completing of the drainage works [24].

Competing Interests

The authors declare that they have no competing interests.

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