Identification of Parameters of the Basic Hydrophysical Characteristics of Soil

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Abstract

The problem of determining parameters of the basic hydrophysical characteristics is studied. These parameters are defined by the type of the soil. To determine these parameters, a model of unsaturated water flow in porous media is considered. The modeled values of soil moisture at various depths are obtained as a result of solution of the initial boundary values problem for Richards equation. The parameters identification problem is stated as an optimal control problem. The objective function is mean-square deviation of simulated values of soil moisture at various points from some prescribed values. Discretized problem is proposed to solve by Marquardt-Levenberg method.

1 Introduction

Models of water transfer in soils play an important role in modeling runoff in the catchment area.The hydrophysical characteristics of soil included in these models are calculated, as a rule, by van Genuchten formulas [van Genuchten, 1980]. These formulas contain some parameters (VG-parameters). Their determination is not an easy task. The specification of the exact values of these parameters is of critical importance in modeling and predicting water flow and transfer of dissolved substances in the aeration zone. This problem has been studied by many authors. Various optimization methods were applied to obtain values of these parameters. Computer programs have been developed to determine these parameters. Here it should be noted the computer program RETC [van Genuchten et al., 1991], allowing among other things to determine them from the measured function of water retention, as well as the program Rosetta [Scaap et al., 2001] which allows in particular to determine hydrological parameters with the help of pedotransfer functions obtained by neural networks. In [Pan & Wu, 1998], a hybrid algorithm based on simulated annealing was used in searching values of hydraulic

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parameters. In [Takeshita, 1999], [Vrugt et al., 2001] the parameters were obtained by genetic algorithm. Over the past decades, to determine the parameters, many authors have applied the methods imitating the behavior of biological populations in conditions of lack of vital resources and migrating in order to find a place with favorable living conditions, algorithms imitating social behavior, see, for example, [Abbaspourt et al., 2001], [Yang & You, 2013].

In the present paper the parameter identification problem is stated as an optimal control problem in which the control is unknown parameters, and the objective function is mean-square deviation of calculated values of soil moisture at various depths from some prescribed values. Calculation of soil moisture is performed in according to the model of water transfer in soil. As a result of finite difference approximation, the problem is reduced to nonlinear programming problem. Numerical solution is obtained by Marquardt-Levenberg method. Jacobian of the moisture function is calculated by formulas of fast automatic differentiation [Aida-Zade & Evtushenko, 1989], [Griewank & Corliss, 1999], [Evtushenko, 1991], [Evtushenko, 1998].

2 Problem Formulation

Consider an one-dimensional model of vertical water transfer in soil. Suppose that soil is homogeneous isothermal non-deformable porous media. Under these assumptions vertical water transfer in soil is well described by one-dimensional nonlinear second order parabolic partial differential equation. Consider following initial boundary value problem:

$$\begin{aligned}
&\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial z}\left(D(\theta)\frac{\partial\theta}{\partial z}\right)-\frac{\partial K(\theta)}{\partial z}, \quad (z,t)\in Q,\\
&\theta(z,0)=\varphi(z), \quad z\in(0,\mathrm{L}),\\
&\theta(L,t)=\psi(t), \quad t\in(0,T),\\
&-\left(D(\theta)\frac{\partial\theta}{\partial z}-K(\theta)\right)\Big|_{z=0}=R(t)-E(t), \quad t\in(0,T),\\
&\theta_{min}\le\theta(0,t)\le\theta_{max}, \quad t\in(0,T),
\end{aligned} \tag{1}$$

where z is space variable; t is time; $\theta(z,t)$ is soil moisture at the point (z,t); $Q=(0,L)\times(0,T)$; $\varphi(z)$ and $\psi(t)$ are given functions; $D(\theta)$ and $K(\theta)$ are diffusion coefficient and hydraulic conductivity – the hydrophysical characteristics of the soil; $\theta_{min}=\theta_r+\varepsilon$ and $\theta_{max}=\theta_s-\varepsilon$, where θ_r and θ_s are, respectively, the residual moisture and the saturation moisture depending on the soil type, and ε is a constant such that $0<\varepsilon\ll\theta_r$; $R(t)$ is precipitation; $E(t)$ is evaporation, $0\le E(t)\le M$, $t\in(0,T)$, M is a constant such that $M>0$.

The diffusion coefficient $D(\theta)$ and the hydraulic conductivity $K(\theta)$ appearing in this equation are found by the widely used van Genuchten formulas [van Genuchten, 1980]

$$\begin{aligned}
&K(\theta)=K_0S^{0.5}[1-(1-S^{1/m})^m]^2,\\
&D(\theta)=K_0\frac{1-m}{\alpha m(\theta_s-\theta_r)}S^{0.5-1/m}\times[(1-S^{1/m})^{-m}+(1-S^{1/m})^m-2],
\end{aligned} \tag{2}$$

where $S=\dfrac{\theta-\theta_r}{\theta_s-\theta_r}$; and K_0, α, m are some parameters. Described problem (1)-(2) will be called the direct problem.

Formulate the parameters identification problem. Let a function $\hat{\theta}(z,t)$ be defined on some set $Q_0\subseteq Q$. Call this function $\hat{\theta}(z,t)$ "experimental data". Introduce a set $U=\{u:u\in R^3;0\le a[i]\le u[i]\le b[i],i=\overline{1,3}\}$. Denote $[K_0,\alpha,m]^T$ by u. The problem is to pick up the parameters K_0, α and m in such a way that corresponding solution of the direct problem (1)-(2) is as close as possible to the function $\hat{\theta}(z,t)$ on the set Q_0. More precisely, the problem is to find u^{opt}, $u^{opt}\in U$, and corresponding solution $\theta^{opt}(z,t)$ of the direct problem (1)-(2) which minimize functional

$$J=\frac{1}{2}\int_{Q_0}(\theta-\hat{\theta})^2dzdt.$$

3 Discretization of the Direct Problem

To approximate the direct problem (1)-(2 by finite differences we divide the intervals $(0,T)$ and $(0,L)$ into N and I equal subintervals with the endpoints $t^n=\tau n$, $0\le n\le N$, and $z_i=hi$, $0\le i\le I$, correspondingly, where $\tau=T/N$ $h=L/I$. Approximate the direct problem (1)-(2 by following finite differences scheme:

$$\frac{\theta_i^{n+1} - \theta_i^n}{\tau} = \frac{1}{h} \left(D_{i+1/2}^{n+1} \frac{\theta_{i+1}^{n+1} - \theta_i^{n+1}}{h} - K_{i+1/2}^{n+1} - D_{i-1/2}^{n+1} \frac{\theta_i^{n+1} - \theta_{i-1}^{n+1}}{h} + K_{i-1/2}^{n+1} \right),$$

$$1 \le i < I; \quad 0 \le n < N,$$

$$\theta_i^0 = \varphi_i, \quad 0 \le i \le I, \quad \theta_I^n = \psi^n, \quad 1 \le n \le N.$$

Here θ_i^n, $D_{i+1/2}^n$, $K_{i-1/2}^n$ are values of the functions $\theta(z,t)$, $D(\theta(z,t))$, $K(\theta(z,t))$ at the points $(ih, n\tau)$, $((i+1/2)h, n\tau)$, $((i-1/2)h, n\tau)$, correspondingly.

Approximate the left boundary condition in the form

$$\frac{\theta_0^{n+1} - \theta_0^n}{\tau} = \frac{2}{h} \left(D_{1/2}^{n+1} \frac{\theta_1^{n+1} - \theta_0^{n+1}}{h} - K_{1/2}^{n+1} + R^{n+1} - E^{n+1} \right), \qquad 0 \le n < N,$$

where R^{n+1}, E^{n+1} are values of functions $R(t)$ and $E(t)$ at the points $t = (n+1)\tau$.

Thus, the discrete analog of the direct problem (1)-(2 has a form

$$\begin{gathered}
\Phi_0^n = -\left(\frac{1}{\tau} + \frac{2}{h} D_{1/2}^n \right) \theta_0^n + \frac{2}{h} D_{1/2}^n \theta_1^n + \frac{1}{\tau} \theta_0^{n-1} + \frac{2}{h} \left(-K_{1/2}^n + R^n - E^n \right) = 0, \\
\theta_{min} \le \theta_0^n \le \theta_{max}, \quad 1 \le n \le N, \\
\Phi_i^n = \frac{1}{h^2} D_{i-1/2}^n \theta_{i-1}^n + \frac{1}{h^2} D_{i+1/2}^n \theta_{i+1}^n - \left\{ \frac{1}{\tau} + \frac{1}{h^2} \left(D_{i+1/2}^n + D_{i-1/2}^n \right) \right\} \theta_i^n + \\
+ \left\{ \frac{\theta_i^{n-1}}{\tau} + \frac{1}{h} \left(K_{i-1/2}^n - K_{i+1/2}^n \right) \right\} = 0, \quad 1 \le i \le I-1, \quad 1 \le n \le N, \\
\Phi_I^n = \theta_I^n - \psi^n = 0, \quad 1 \le n \le N, \\
\theta_i^0 = \varphi_i, \quad 0 \le i \le I.
\end{gathered} \tag{3}$$

The diffusion coefficient and the hydraulic conductivity at the intermediate points appearing in formulas (3) are calculated by the formulas

$$D_{i+1/2}^n = \frac{D_i^{n-1} + D_{i+1}^{n-1}}{2}, \quad K_{i+1/2}^n = \frac{K_i^{n-1} + K_{i+1}^{n-1}}{2}, \qquad 1 \le n \le N, \quad 0 \le i < I. \tag{4}$$

4 Discrete Optimal Control Problem

Introduce a set $Q_0 = \{(z,t) : z = ih, t = l\tau, (i,l) \in A\}$, where $A = \{(i,l) : i = 0, 1, \ldots, I, \ l = 1, \ldots, d\}$, where $0 < d \le N$, d is some natural number. Denote vector of desirable parameters by u, $u \in U$, where $U = \{u : u \in R^3, 0 < a[i] \le u[i] \le b[i], i = \overline{1,3}\}$. Define the objective in the form

$$W(\theta, u) = \frac{1}{2} \sum_{(j,n) \in A} \left(\theta_j^n - \hat{\theta}_j^n \right)^2 \tau h. \tag{5}$$

The optimal control problem is to find optimal control $u^{opt} \in U$ and corresponding optimal solution $\theta^{opt}(z,t)$ of the direct problem (3)-(4) that minimize the objective function $W(\theta, u)$ (5).

Earlier in ([Zasukhina & Zasukhin, 2017]), the problem of the identification of two parameters α and m was investigated. The problem was considered in the same formulation. In particular, the optimal control problem with the objective function (5) with various d was studied. Numerical solution of the problem was curried out using steepest descent method. Exact gradient of the objective function was calculated by formulas of fast automatic differentiation (FAD). As calculation experiments showed, for the values of d from 8 to 10, the obtained parameters α and m differ from their true values by 0.4% and 0.1% respectively.

Here we tried to determine three parameters using steepest descent method. But these attempts have encountered difficulties. The obtained parameters differed from the true ones very significantly. For this reason another algorithm of numerical optimization was applied.

Due to the form of the objective function, Levenberg–Marquardt algorithm [Levenberg, 1944], [Marquardt, 1963] of numerical optimization can be applied to the solution of the considered optimal control problem. This method is a combination of the Gauss-Newton algorithm with gradient descent method. And in this case, the exact values of the Jacobian of the soil moisture function $[\theta_0^1, \theta_1^1, \ldots, \theta_I^1, \ldots, \theta_0^N, \theta_1^N, \ldots, \theta_I^N]^T$ is proposed also to be calculated using FAD method.

4.1 Optimization by Levenberg-Marquardt Algorithm

We rewrite the objective function in the form

$$W(\theta, u) = \sum_{(j,n)\in A} \left(\theta_j^n - \hat{\theta}_j^n\right)^2, \tag{6}$$

where $A = \{(i,l) : i = 0, 1, \ldots, I, \ \ l = 1, \ldots, d\}$, d is some natural number, $d \leq N$. Denote $[\theta_0^1, \theta_1^1, \ldots, \theta_I^1, \ldots, \theta_0^N, \theta_1^N, \ldots, \theta_I^N]^T$ and $[\hat{\theta_0^1}, \hat{\theta_1^1}, \ldots, \hat{\theta_I^1}, \ldots, \hat{\theta_0^N}, \hat{\theta_1^N}, \ldots, \hat{\theta_I^N}]^T$ by Θ and $\hat{\Theta}$ respectively. According to the Levenberg–Marquardt optimization algorithm at each iteration step k, the displacement vector $\Delta(u_k)$ is determined from following system of equations:

$$(J(u_k)^T J(u_k) + \lambda \mathrm{diag}(J^T(u_k) J(u_k)) \Delta u_k = -J^T(u_k)(\Theta - \hat{\Theta}),$$

where $J(u_k)$ is the Jacobian of the function $\Theta(u_k)$:

$$J = \begin{pmatrix} \dfrac{\partial \theta_0^1}{\partial u^1} & \cdots & \dfrac{\partial \theta_I^1}{\partial u^1} & \cdots & \dfrac{\partial \theta_0^N}{\partial u^1} & \cdots & \dfrac{\partial \theta_I^N}{\partial u^1} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \dfrac{\partial \theta_0^1}{\partial u^3} & \cdots & \dfrac{\partial \theta_I^1}{\partial u^3} & \cdots & \dfrac{\partial \theta_0^N}{\partial u^3} & \cdots & \dfrac{\partial \theta_I^N}{\partial u^3} \end{pmatrix}^T . \tag{7}$$

The parameter λ is positive and may be adjusted at the each iteration. The Jacobian of $\Theta(u)$ is proposed to be calculated using FAD formulas.

5 Fast Automatic Differentiation Method

Fast automatic differentiation method allows to compute derivatives of complex functions whose variables are related by functional relationships. Briefly describe the essence of this method.

Let for vectors $z \in R^n$ and $u \in R^r$ continuously differentiable functions $F(z, u)$ and $G(z, u)$ define mappings $F : R^n \times R^r \longrightarrow R^1$ and $G : R^n \times R^r \longrightarrow R^n$. Let z and u satisfy the system of n scalar algebraic equations

$$G(z, u) = 0_n, \tag{8}$$

where 0_n is zero n-dimensional vector. Suppose that the matrix $G_z^T(z, u)$ is not singular. We denote the matrix transposed to the matrix $G_z(z, u)$ by $G_z^T(z, u)$. Then according to the implicit function theorem, the relations (8) define continuously differentiable function $z = z(u)$. And according to FAD method, the gradient of the function $F(z(u), u)$ is calculated by following formula:

$$dF(z(u), u)/du = F_u(z(u), u) + G_u^T(z(u), u)p. \tag{9}$$

The vector $p \in R^n$ from this formula is Lagrange multiplier which is determined as a result of the solution of following linear system of equations :

$$F_z(z(u), u) + G_z^T(z(u), u)p = 0_n. \tag{10}$$

The system (10) is linear with respect to p and adjoint to the initial system (8).

Thus, in accordance with the formulas (8)-(10), we obtain the relations for computing gradient of $V = \theta_i^n$, $i = \overline{0, I}$, $n = \overline{1, N}$

$$dV(\theta(u), u)/du = V_u(\theta(u), u) + \Phi_u^T(\theta(u), u)p, \tag{11}$$

$$V_\theta(\theta(u), u) + \Phi_\theta^T(\theta(u), u)p = 0_L, \tag{12}$$

where $\Phi^T = [\Phi_0^1, \Phi_1^1, \ldots, \Phi_I^1, \Phi_0^2, \Phi_1^2, \ldots, \Phi_I^2, \ldots, \Phi_0^N, \Phi_1^N, \ldots, \Phi_I^N]$, $p \in R^L$ is Lagrange multiplier, $u \in U \subset R^3$, $\theta^T = [\theta_0^1, \theta_1^1, \ldots, \theta_I^1, \theta_0^2, \theta_1^2, \ldots, \theta_I^2, \ldots, \theta_0^N, \theta_1^N, \ldots, \theta_I^N]$, $L = (I + 1)N$.

6 Numerical Results

Described approach was applied to finding the numerical solution of the discrete optimal control problem. The problem was solved with following values of input parameters:

$$
\begin{aligned}
&L = 100(\text{cm}), \quad T = 1(\text{d}), \quad \theta_{min} = 0.05(\text{cm}^3/\text{cm}^3), \quad \theta_{max} = 0.5(\text{cm}^3/\text{cm}^3),\\
&\varphi(z) = 0.3, \quad z \in (0, L), \qquad \psi(t) = 0.3, \quad t \in (0, T), \quad a = [0, 0.005, 0.01]^T, \quad b = [300, 0.1, 0.5]^T.
\end{aligned}
$$

The grid with $I = 100$ and $N = 96$ was used. The calculations were curried out in three stages.

6.1 The First Stage of Calculations

At this stage, the direct problem (3)-(4) with the parameters $K_0^{true} = 100(\text{cm/d})$, $\alpha^{true} = 0.01$ and $m^{true} = 0.2$ was solved. It is clear from the form of the system (3) and formulas for diffusion coefficient and hydraulic conductivity at intermediate points (4) that the system (3) can be split into N subsystems which of them corresponds to certain time layer. Each subsystem can be solved independently from others subsystems. For each such subsystem, the basic matrix is tridiagonal. Therefore, each subsystem was solved by tridiagonal matrix algorithm. Obtained solution was taken as a prescribed function $\hat{\theta}(z, t)$.

6.2 The Second Stage of Calculations

At the second stage the numerical solution of the optimal control problem was searched by steepest descent method. Exact gradient of the objective function (5) was calculated by formulas of FAD. Step value along the chosen direction was determined as a result of procedure of one-dimensional optimization along this direction of the function interpolating the objective function by means of splines constructed on 40 points. We considered the optimal control problems with the objective function (5), where d varied from 1 to 10. For all problems numerical optimization was curried out with various initial approximations. Each initial approximation differed one from another by value of the first component, namely initial approximations for α and m were equal to 0.03 and 0.13 correspondingly and K_0^{init} was equal to 102, 105, 110, 120, 150, 180, 200.

Numerical calculations showed that for each initial approximation, the results improve slightly with increasing d from 1 to 10. At the same time, the deviation of the obtained values of the parameters α^{opt} and m^{opt} from the true values α^{true} and m^{true} depends on the initial approximation. So, with the change of K_0^{init} from 102 to 200, this deviation varies from 1.1% to 44.7% for α and – from 0.25% to 8.2% for m.

As to the parameter K_0, its value does not practically change during the optimization process and remains very close to the initial value. And, the further the initial approximation of the parameter K_0 from its true value, the smaller the difference between the initial value and the obtained value of the parameter K_0. This difference does not exceed $1.44 \cdot 10^{-5}$. Presumably, this inability of K_0 to be optimized is due to the fact that the corresponding component of the gradient of the objective function differs from other components by 3-4 orders of magnitude.

The values of the parameters K_0^{opt}, α^{opt} and m^{opt} obtained for various initial approximations are presented in Figure 1. Under various initial approximations, we mean that the value of K_0^{init} changes, while the values of α^{init} and m^{init} remain unchanged. The graphs, following from left to right in Figure 1, refer to K_0^{opt}, α^{opt} and m^{opt} correspondingly. These graphs are designated by solid line. Dashed line shows true values of the parameters.

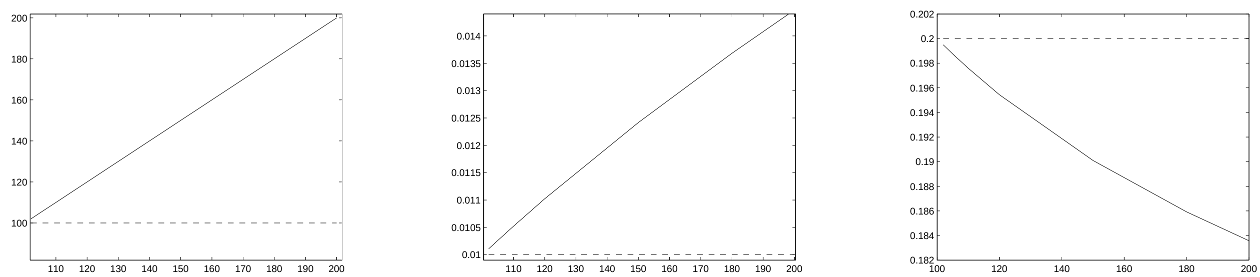

Figure 1: Dependencies of Obtained Parameters on Initial Approximation

Thus, these numerical calculations showed that the application of the steepest descent method to solving K_0, α, m identification problem does not lead to satisfactory results.

6.3 The Third Stage of Calculations

As the numerical experiments at the second stage showed, to identify parameters K_0, α and m with good accuracy, another (not the steepest descent method) algorithm should be applied. Therefore, in order to solve the discrete optimal control problem, the Levenberg-Marquardt algorithm was applied. The objective function was defined by formula (6), where $A = \{(j,n) : j = \overline{0,I}, n = 1,\dots,d\}$. The cases of $d = 2,3,4,5,6,7,8,9,10$ were considered. At each iteration in determining the direction of the search, the exact derivatives of θ_j^n, $n = \overline{1,N}$, $j = \overline{0,I}$, were calculated using FAD formulas (11)-(12). The process of the numerical optimization started with initial approximation $K_0^{init} = 200$, $\alpha^{init} = 0.03$ and $m^{init} = 0.13$. The parameter λ changed during the process of numerical optimization. At the beginning it was equal, as a rule, to 10^{-4} and then it was adjusted at each iteration. The process of the numerical optimization continued until the Chebyshev norm of the gradient of the objective function became less than $1.1{\cdot}10^{-18}$ and value of the objective function became less than $2{\cdot}10^{-24}$. The results of the calculations are presented in following table:

Table 1: Obtained Values of Parameters K_0, α and m

d	K_0^{opt}	Error	α^{opt}	Error	m^{opt}	Error	gradient	function
2	100.21	0.21%	$1.0011 \cdot 10^{-2}$	0.11%	$1.9995 \cdot 10^{-1}$	0.03%	$9.16{\cdot}10^{-20}$	$1.92{\cdot}10^{-24}$
3	100.09	0.09%	$1.0005 \cdot 10^{-2}$	0.05%	$1.9998 \cdot 10^{-1}$	0.01%	$1.08 \cdot 10^{-18}$	$1.02 \cdot 10^{-25}$
4	100.09	0.09%	$1.0005 \cdot 10^{-2}$	0.05%	$1.9998 \cdot 10^{-1}$	0.01%	$8.22 \cdot 10^{-21}$	$3.71 \cdot 10^{-26}$
5	100.19	0.19%	$1.0010 \cdot 10^{-2}$	0.10%	$1.9995 \cdot 10^{-1}$	0.03%	$6.41 \cdot 10^{-21}$	$6.78 \cdot 10^{-26}$
6	100.06	0.06%	$1.0003 \cdot 10^{-2}$	0.03%	$1.9998 \cdot 10^{-1}$	0.01%	$2.34 \cdot 10^{-19}$	$3.40 \cdot 10^{-27}$
7	100.001	0.001%	$1.00001 \cdot 10^{-2}$	0.001%	$1.999997 \cdot 10^{-1}$	0.0002%	$5.22 \cdot 10^{-20}$	$7.30 \cdot 10^{-31}$
8	100.03	0.03%	$1.0002 \cdot 10^{-2}$	0.02%	$1.99992 \cdot 10^{-1}$	0.004%	$2.33 \cdot 10^{-19}$	$2.21 \cdot 10^{-28}$
9	100.008	0.008%	$1.00004 \cdot 10^{-2}$	0.004%	$1.99998 \cdot 10^{-1}$	0.001%	$2.46 \cdot 10^{-19}$	$1.05 \cdot 10^{-29}$
10	100.002	0.002%	$1.000008 \cdot 10^{-2}$	0.0008%	$1.999996 \cdot 10^{-1}$	0.0002%	$1.38 \cdot 10^{-19}$	$2.25 \cdot 10^{-31}$

It can be seen from Table 1 that optimal values of the parameters K_0, α and m are getting closer to their true values as d increases from 2 to 10. So, while d increases from 2 to 10, the deviation of K_0^{opt} from K_0^{true} decreases from 0.21% to 0.002%, the deviation of α^{opt} from α^{true} decreases from 0.11% to 0.0008%, and the deviation of m^{opt} from m^{true} decreases from 0.03% to 0.0002%. The time required to find the solution turned out to be approximately the same for all problems considered.

The value of d defines the set where measured and calculated values of soil moisture are compared. Therefore, the choice of d defines initial data required for determining the parameters. Thus, analyzing results of the numerical calculation, we can estimate how choice of one or another set of initial data will influence on the accuracy of the solution obtained.

Conclusion

Analysis of the results of the numerical calculations leads us to following conclusion.

- The application of the Levenberg-Marquardt method to solving parameters identification problem allows to determine these parameters with good accuracy. So, we can determine the parameter K_0 with accuracy up to 0.002%, the parameter α – up to 0.0008% and the parameter m^{opt} – up to 0.0002%.

- The gradient method turned out to be ineffective in determining three parameters K_0, α and m. In particular, the difficulties in solving this problem are due to the fact that one component of the gradient of the objective function differs from the other components by 3-4 orders of magnitude.

It should be noted the disadvantage of the proposed approach: the Levenberg-Maquardt algorithm used in the process of numerical optimization is one of the local methods. And therefore, there is the question of the possibility of applying in this situation a method of global optimization, for example, of the well-known uneven coating method [Evtushenko & Posypkin, 2013].

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