SIMULTANEOUS ESTIMATION OF HYDRODIPERSIVE PARAMETERS USING A NEW MODIFIED LEVENBERG–MARQUARDT ALGORITHM

H. QANZA, A. MASLOUHI, M.HACHIMI, A.HMIMOU
Department of Physics, Interdisciplinary Laboratory for Natural Resources
and Environment, Ibn Tofail University, Kenitra, Morocco,
hqanza@gmail.com
maslouhi_a@yahoo.com

Abstract
Determination of soil hydrodynamic parameters at field scale is of great importance for modeling soil water dynamics and for agricultural water management. The direct estimation of those parameters is time-consuming and afflicted with serious uncertainties. Inverse modeling is known to get efficient technique for solving non-linear problems in hydrology. Levenberg–Marquardt (LM) algorithm is a gradient-based method, which has been widely used for solving inverse soil water flow problems. In LM algorithm, sensitivity coefficients are mainly evaluated by numerical differentiation methods. However, sensitivity coefficients are difficult to be precisely calculated by numerical differentiation methods, if transient states and non-linearities are involved. In this paper, a new approach is proposed for sensitivity analysis using complex variable-differentiation method (CVDM) to estimate simultaneously the hydraulic and dispersive properties of unsaturated soil from in-situ experiments. In this approach, the sensitivity coefficients can be determined in a more accurate way than the traditional finite difference method. The results show that the new inverse analysis method in the present work has the high accuracy, validity, uniqueness and higher inversion efficiency, compared with the previous least-squares method. The simulated and measured water contents and tracer concentration were generally close. Overall, it was concluded that the CVDM is promising method to estimate hydro-dispersive parameters in unsaturated zone.

Keywords : *Unsaturated soil, Hydro-dispersive parameters; Inverse modeling; Levenberg–Marquardt; Complex-variable-differentiation*

1. Introduction
Modeling of water and solute transport in soil systems is often done by numerical simulations, based on the Richards equation. To obtain reliable simulation results, exact knowledge of the soil hydraulic properties at the scale of interest is indispensable [1]. This is problematic, because predictions of water and solute transport for hydrologic management decisions are generally needed at larger scales such as the field scale, whereas these proprieties are usually determined in the laboratory on small soil cores. Due to spatial variability and high non-linearity of soil hydraulic proprieties, these were often found to be inadequate for describing water dynamics at larger spatial scales. An alternative is to use observations made at the scale of interest under known boundary conditions and to estimate system parameters by inverse modeling [2]. A popular inverse method used in soil physics combines the numerical model with an algorithm for parameter estimation [3]. Basically, the process aims at the best parameters set iteratively, by varying the parameters and comparing the real response of the system measured with the numerical solution. Indeed, the search should consist of finding the global minimum of an objective function which is defined by the error between measured and simulated values. Levenberg–Marquardt (LM) algorithm [4] is a gradient-based method, which has been widely used for solving inverse soil water flow and solute transport problems. In a traditional LM algorithm, sensitivity coefficients are mainly evaluated by numerical differentiation methods. However, sensitivity coefficients are difficult to be precisely calculated by these methods, if multi-parameters, transient states and nonlinearities are involved. In this study, we present a modified LM algorithm. In this algorithm, we introduce the complex variable differentiation method (CVDM) into the conventional LM algorithm, within which the sensitivity coefficients are precisely calculated, rather than using numerical differentiation method in conventional LM. CVDM was first described mathematically by Lyness and Moler [5]. CVDM applications in many area has offered a great improvement in accuracy over finite differentiation. Our solution follows the methodology outlined by paper of Cui (2016) [6] for heat conduction problems.

Despite mathematical specificities of the above equations (Richards and transport equations), we showed that the CVDM method worked very well and presented certain advantages over classical methods. To the best of our knowledge, this is the first application of the CVDM in the soil physics area with real field conditions.

2. Mathematical models

2.1 Direct modeling

The one-dimensional movement of water in soil is described by the Richards' equation:

$$C(h)\frac{\partial h(z,t)}{\partial t}=\frac{\partial}{\partial z}\left[K(h)\frac{\partial h(z,t)}{\partial z}-K(h)\right]-\frac{E}{Z_e} \qquad (1)$$

Where : h is the water pressure head (cm), $C(h)=\partial\theta/\partial h$, is called the specific moisture capacity function with θ is water content, t is time (s), z is the vertical space coordinate (cm) (positive upward), K is the hydraulic conductivity function (cm s^{-1}), E is the actual evaporation (L T^{-1}), and Z_e is the depth affected by evaporation [7].

Richard's equation is coupled with solute transfer model described by the advection-dispersion equation:

$$\frac{\partial(\theta c)}{\partial t}=\frac{\partial}{\partial z}\left(\theta D\frac{\partial c}{\partial z}\right)-\frac{\partial(qc)}{\partial z} \qquad (2)$$

Where : C (g cm^{-3}) is the concentration of bromide; $D=\lambda.\upsilon$ (cm^2 s^{-1}) is the coefficient of hydrodynamic longitudinal dispersion. υ : the pore water velocity $\upsilon=q/\theta$ (cm s^{-1}).

2.2 Inverse modeling by complex variable-differentiation method

The inverse optimization procedure is usually performed using a least squares criterion with respect to some objective function. Mathematically, it is generally formulated as follows[8]:

$$S(p_k,y)=\sum_{i}^{nz}\sum_{j}^{nt}\sigma_i^j\,(y_i^j(z,p_k)-y_{i,mes}^j)^2 \qquad (3)$$

where n_z is the number of measurements, n_t the number of time steps, $\sigma_i=(y_{mes,min}-y_{mes,max})^{-2}$ is the measurement weighting, y_i and $y_{i,mes}$ are model predictions and observations respectively.

The Levenberg–Marquardt algorithm (LM) is adopted for minimizing the objective function in Eq.(3). The inverted parameters vector is given by Eq.(4).

$$\Delta p_k^{(m)}=-(J^T(p_k^{(m)}).w.J(p_k^{(m)})+\gamma.I)^{-1}G(p_k^{(m)}) \qquad (4)$$

Where: $J=\partial y(p_k)/\partial p_k$ is the sensitivity coefficients matrix, $G(p_k)$ is the gradient vector of objective function, γ is the damping factor, I is a diagonal scaling matrix.

It can be seen that accurately evaluating sensitivity coefficients in Eq. (4) is very important for a LM algorithm.

Recently, the first author and co-authors have presented a modified LM algorithm for estimating hydro-dispersive parameters in Ref. [9], in which, the sensitivity coefficients are accurately determined by using the complex-variable-differentiation method (CVDM) [6-9]. In this approach the CVDM gives a very simple expression for estimating the first derivative. This procedure uses an imaginary step to approximate the first derivative and avoids subtractive error cancellation in finite difference approximation.

In CVDM, the variable x of a real function F(x) is replaced by the complex variable x+iη, with the imaginary part η being very small. The function F(x+iη) can be expanded in a Taylor series as:

$$F(x+i\eta)=F(x)+i\eta F'(x)-\frac{\eta^2}{2}F''(x)+o(\eta^3),\forall x\in\Re \qquad (5)$$

where η is a small positive real step and i is the imaginary. Taking imaginary parts on both sides, we obtain:

$$\mathrm{Im}[F(x+i\eta)]=\eta F'(x)-\eta^3\frac{F'''(x)}{3!}+..., \qquad (6)$$

from where we can finally write:

$$\begin{aligned}F'(x)&=\frac{\mathrm{Im}[F(x+i\eta)]}{\eta}+\eta^2\frac{F'''(x)}{3!}+...\\&=\frac{\mathrm{Im}[F(x+i\eta)]}{\eta}+O(\eta^2)\end{aligned} \qquad (7)$$

Thus to within second-order the complex-variable derivative approximation of F is given by:

$$F'(x)\approx\frac{\mathrm{Im}[F(x+i\eta)]}{\eta} \qquad (8)$$

3. Results and discussion

The direct simulation is performed with the VZM code[10] (developed by Saadi and Maslouhi, 2003).The analysis of the evolution of the water content helps to understand the spatial and temporal aspects of water transfers.

The CVDM was employed to estimate model parameters in Eqs.(1) and (2), where only information on water content and bromide concentration data was incorporated in the objective functions. This is done to identify hydro-dispersive parameters. The optimization started with the same initial guesses for model parameters (θ_r= 0 cm^3 cm^{-3}, θ_s= 0.39 cm^3 cm^{-3}, α= 0.20 cm^{-1}, k_s=5.10^{-3} cm s^{-1}, n= 2 and λ= 11.5 cm). The search continued until the termination criterion was fully satisfied. The convergence curves by using the conventional LM algorithm are shown in Fig.1(a), Fig.1(b), Fig.1(c) and Fig.1(d), in which the convergences are achieved after 23 iterations . In addition, each optimized parameter is converged to its real value, although sensitivity coefficients are not accurately calculated by using the conventional LM algorithm especially for k_s parameter. We conclude from Fig.1 that the modified LM algorithm keeps the advantage of high accuracy of the conventional LM algorithm to estimate hydrodynamic parameters. Table 1 summarizes the average optimized hydro-dispersive parameters from inverse modeling. An effective result for each parameter is given by statistic indexe RMSE. Meanwhile, the efficiency of the modified LM algorithm is improved compared with the conventional LM algorithm, which is attributed to accurate evaluation of sensitivity coefficients. One has to be at the expense of low efficiency by using the conventional LM algorithm, even though a convergence can be achieved if Δp_k is given a suitable value. In addition, the modified LM algorithm is independent of the step size Δp_k, if Δp_k is small enough. However, it is different for the conventional LM algorithm, in which the inverse analysis is affected by the step size Δp_k, and divergence will occur as η decreases. This implies the modified LM algorithm is more stable than the conventional LM algorithm.

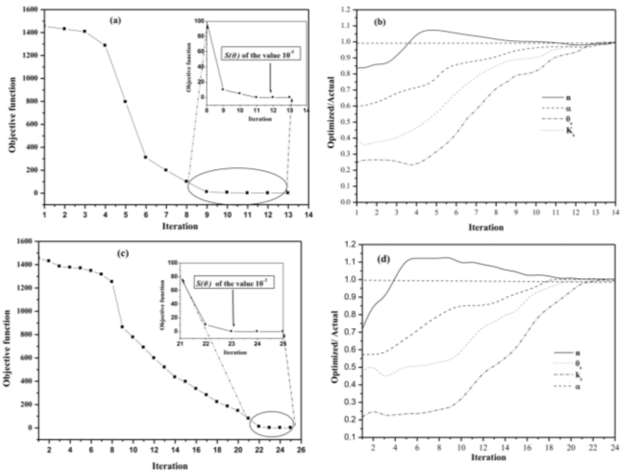

Figure 1. Convergence curves by using modified LM algorithm (a):*S(θ),* (b) reduced parameters and by using the conventional LM algorithm: (c) *S(θ),* (d) reduced parameters.

Table 1. Results of hydro-dispersive parameters obtained by the conventional and the modified LM.

Parameter	Initial value	Estimated value by LM algorithm	RMSE	Estimated value by using CVDM	RMSE
θ_r (cm^3/cm^3)	0	0.017	0.02	0.019	0.013
θ_s (cm^3/cm^3)	0.39	0.428		0.43	
n (-)	2.00	2.191		1.86	
α (cm^{-1})	0.20	0.330		0.365	
k_s (cm s^{-1})	5.10^{-3}	0.0077		0.0079	
λ (cm)	11.5	8.9		8.11	

4. Conclusions

In the present work, a modified LM algorithm is applied for simultaneous estimation of hydro-dispersive parameters of water flow and solute transfer problems in unsaturated soils, in which the complex-variable-differentiation method is introduced for accurate evaluation of hydro-dispersive properties with their sensitivities coefficients. The result shows that the modified LM algorithm has the advantages of the conventional LM algorithm that are effective, accurate and robust for simultaneous estimation of hydro-dispersive parameters. Meanwhile, the efficiency and the convergence stability of the modified LM algorithm are improved, compared with the conventional LM algorithm. Further, the combining the direct model and the modified LM algorithm proved to be a useful tool to calculate the hydro-dispersive properties of unsaturated soils.

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