The DISC Computer Software for Analyzing Tension Disc
Infiltrometer Data by Parameter Estimation

Version 1.0

Research Report No. 145

January 2000

U. S. SALINITY LABORATORY

AGRICULTURAL RESEARCH SERVICE

U. S. DEPARTMENT OF AGRICULTURE

RIVERSIDE, CALIFORNIA

The DISC Computer Software for Analyzing Tension Disc

Infiltrometer Data by Parameter Estimation

Version 1.0

by

Jiří Šimůnek and M. Th. van Genuchten

Research Report No. 145

January 2000

U. S. SALINITY LABORATORY

AGRICULTURAL RESEARCH SERVICE

U. S. DEPARTMENT OF AGRICULTURE

RIVERSIDE, CALIFORNIA

DISCLAIMER

This report documents version 1.0 of DISC, a software package for estimating the unsaturated soil hydraulic properties from tension disc infiltration data and related information. The software has been verified against a large number of test cases. However, no warranty is given that the program is completely error-free. If you do encounter problems with the code, find errors, or have suggestions for improvement, please contact one of the authors at

U. S. Salinity Laboratory
USDA, ARS
450 West Big Springs Road
Riverside, CA 92507

Tel. 909-369-4865 (J. Šimůnek)
Tel. 909-369-4846 (M. Th. van Genuchten)
Fax. 909-342-4964
E-mail jsimunek@ussl.ars.usda.gov
        rvang@ussl.ars.usda.gov

ABSTRACT

Šimůnek, J. and M. Th. van Genuchten. 2000. The DISC Computer Software for Analyzing Tension Disc Infiltrometer Data by Parameter Estimation, Version 1.0, Research Report No. 145, U.S. Salinity Laboratory, USDA, ARS, Riverside, California.

This report documents version 1.0 of DISC, a computer software package for analyzing tension disc infiltrometer data by parameter estimation. The software package consists of the simplified HYDRUS2 computer program, and an interactive graphics-based user interface. The DISC code numerically solves the Richards' equation for saturated-unsaturated water flow. Flow occurs in a three-dimensional region exhibiting radial symmetry about the vertical axis. The software includes a Marquardt-Levenberg type parameter optimization algorithm for inverse estimation of soil hydraulic properties from measured transient cumulative infiltration and related data.

The governing flow equation is solved numerically using Galerkin-type linear finite element schemes. The transport region is discretized automatically by the software into triangular elements using pregenerated files that are scaled directly to the specified size of the tension disc radius.

This report serves as both a user manual and reference document. Detailed instructions are given for data input preparation.

TABLE OF CONTENTS

LIST OF VARIABLES

D	soil water difusivity $[L^2T^{-1}]$
h	pressure head $[L]$
h_i	initial pressure head $[L]$
h_0	time-variable supply pressure head imposed by the tension disc infiltrometer $[L]$
K	hydraulic conductivity $[LT^{-1}]$
K_s	saturated hydraulic conductivity $[LT^{-1}]$
l	pore-connectivity parameter $[-]$
m	empirical shape parameter in the retention curve $(= 1 - 1/n)$ $[-]$
n	empirical shape parameter in the retention curve $[-]$
n_j	number of measurements in a particular measurement set
$q_j^*(t_i)$	specific measurement at time t_i for the jth measurement set
$q_j(t_i, \beta)$	corresponding model predictions for parameter vector β
r	radial coordinate $[L]$
r_0	disc radius $[L]$
S_e	effective fluid saturation $[-]$
t	time $[T]$
v_j	weights associated with a particular measurement set j
w_{ij}	weights associated with a measurement i within set j
z	vertical coordinate $[L]$ positive downward
α	empirical shape parameter in the retention curve $[L^{-1}]$
α^*	sorptive number $[L^{-1}]$
β	vector of optimized parameters (e.g., θ_r, θ_s, α, n, K_s, and l)
θ	volumetric water content $[L^3L^{-3}]$
θ_i	initial water content $[L^3L^{-3}]$
θ_r	residual water contents $[L^3L^{-3}]$
θ_s	saturated water contents $[L^3L^{-3}]$
σ_j^2	measurement variances
Φ	objective function

x

1. INTRODUCTION

Reliable application of computer models to field-scale flow and transport problems demands a commensurate effort in quantifying a large number of model parameters. As increasingly more complicated flow and transport models are being developed, the accuracy of numerical simulation depends upon the accuracy with which the different model parameters are estimated. Knowledge of the unsaturated soil hydraulic properties is especially important when numerical models are used to simulate variably-saturated water flow and contaminant transport. Such simulations are generally based on the numerical solutions of Richards' equation, which require information about the soil water retention, $\theta(h)$, and unsaturated hydraulic conductivity, $K(h)$, functions, where θ is the water content, K the hydraulic conductivity, and h the soil-water pressure head. Accurate measurement of these hydraulic properties is confounded by the extreme spatial heterogeneity of the subsurface environment. The hydraulic properties frequently also show significant variations in time because of cultivation or other agricultural activities, shrink-swell phenomena of fine-textured soil, the effect of particle dispersion and soil crusting, and changes in the concentration and ionic composition of the soil solution [*van Genuchten and Šimůnek*, 1995].

A variety of laboratory and field methods are available for direct measurement of the hydraulic conductivity, *K*, or the soil water diffusivity, *D*, as a function of the pressure head and/or the water content [*Klute and Dirksen*, 1986; *Green et al.*, 1986]. Most laboratory methods are steady-state procedures based on direct inversion of Darcy's law. Transient methods generally involve some type of approximation, or simplification of the Richards' equation. Popular transient methods include the *Bruce and Klute* [1956] horizontal infiltration method, and various modifications thereof such as the hot-air method and the sorptivity method. Popular field methods include the instantaneous profile method, various unit-gradient type approaches, sorptivity methods associated with ponded infiltration, and the crust method based on steady water flow. While relatively simple in concept, these direct measurement methods have a number of limitations that restrict their use in practice. For example, most methods are very time-consuming because of the need to adhere to relatively strict initial and boundary conditions. This is especially true for field gravity-drainage experiments involving medium- and fine-textured soils or layered profiles. Methods requiring repeated steady-state flow situations or other equilibrium conditions are also tedious, while linearizations and other approximations or interpolations to allow analytic or semi-

analytic inversions of the flow equation introduce additional errors. Finally, information about uncertainty in the estimated hydraulic parameters is not readily obtained using direct inversion methods.

A more flexible approach for solving the inverse problem is the use of parameter optimization methods. Optimization procedures also make it possible to simultaneously estimate the retention and hydraulic conductivity functions from transient flow data [*Kool et al.*, 1987]. Early parameter optimization studies focused primarily on solute transport [e.g., *van Genuchten*, 1981; *Parker and van Genuchten*, 1984]. Starting with the studies of *Zachmann et al.* [1981] and *Dane and Hruska* [1983], parameter estimation methods are now increasingly being used also for estimating the unsaturated soil hydraulic functions. Computer models applicable to laboratory column outflow measurements have been given by *Kool et al.* [1985a,b] and *Parker et al.* [1985] for one-step outflow procedures, and by *van Dam et al.* [1992, 1994] and *Eching and Hopmans* [1993] for multi-step approaches. Considerable attention has also been given to the estimation of soil-hydraulic properties from ponded infiltration experiments [*Russo et al.,* 1991; *Bohne et al,* 1992]. While initially applied mostly to laboratory-type experiments, inverse methods are equally well applicable to field data [*Kool and Parker*, 1988], or some appropriate combination of field and laboratory data. An important advantage of inverse procedures, if formulated within the context of a parameter optimization problem, is that a detailed error analysis of the estimated parameter is more easily implemented. While parameter optimization methods provide several advantages, a number of problems related to computational efficiency, convergence, and parameter uniqueness, remain to be solved, especially when many hydraulic parameters must be estimated simultaneously [*van Genuchten and Leij*, 1992].

Tension disc infiltrometers have recently become very popular devices for in-situ measurement of the near-saturated soil hydraulic properties [*Perroux and White*, 1988; *Ankeny et al.*, 1991; *Reynolds and Elrick*, 1991; *Logsdon et al.*, 1993, among many others]. Thus far, tension infiltration data have been used primarily for evaluating saturated and unsaturated hydraulic conductivities, and for quantifying the effects of macropores and preferential flow paths on infiltration. Tension infiltration data are often used to evaluate the saturated hydraulic conductivity K_s and the sorptive number α^* in *Gardner*'s [1958] exponential model of the unsaturated hydraulic conductivity using *Wooding'*s [1968] analytical solution. Analyses of this type require either two infiltration measurements using two different disc diameters [*Smettem and*

Clothier, 1989], or measurements using a single disc diameter but with multiple tensions [e.g., *Ankeny et al.*, 1991].

Although early-time infiltration data can be used to estimate the sorptivity [*White and Sully,* 1987], and consequently the matrix flux potential, only steady-state infiltration rates are usually used for Wooding-type analyses. We recently suggested using the entire cumulative infiltration curve in combination with parameter estimation to estimate additional soil hydraulic parameters [*Šimůnek and van Genuchten*, 1996, 1997]. From an analysis of numerically generated data for one supply tension experiment we concluded that the cumulative infiltration curve by itself does not contain enough information to provide a unique inverse solution [*Šimůnek and van Genuchten*, 1996]. An infinite number of combinations of the saturated hydraulic conductivity, K_s, and the shape factor n (see equations 6 and 7) can produce almost identical infiltration curves. A similar conclusion was reached earlier by *Russo et al.* [1991] for a one-dimensional ponded infiltration experiment. Hence, additional information about the flow process, such as the water content and/or pressure head measured at one or more locations in the soil profile, is needed to successfully obtain unique inverse solutions for the soil hydraulic functions.

In our more recent paper [*Šimůnek and van Genuchten*, 1997] we studied, again numerically, infiltration resulting from several consecutive supply tensions. We considered different scenarios, each having different levels of information, and concluded that the best practical scenario is to estimate the hydraulic parameters from the cumulative infiltration curve measured at several consecutive tensions applied to the soil surface, in conjunction with knowledge of the initial and final water content. Our results suggest that one should be able to use information typically being collected with a tension disc infiltrometer to estimate not only unsaturated hydraulic conductivities but, without further experiments, also the soil water retention properties.

The above methodology was further tested on data collected as part of the soil hydrology program of the HAPEX-Sahel regional-scale experiment [*Cuenca et al.,* 1997]. We showed [*Šimůnek et al.,* 1998a] that it is indeed possible to obtain relatively reliable estimates of soil hydraulic conductivities for near-saturated moisture conditions from tension disc infiltration data by numerical inversion, consistent with results of the traditional Wooding analysis. However, the question whether or not it is possible to simultaneously estimate also the retention curve was still not resolved satisfactorily.

In this report we describe a computer software package, DISC, that may be used to analyze tension disc infiltrometer data based on the methodology suggested by *Šimůnek and van Genuchten* [1997]. The method uses knowledge of the cumulative infiltration curve and the initial and final water contents to optimize soil hydraulic parameters by fitting measured data. The code is integrated into a Windows based graphics interface that facilitates entering of the input information and display of the parameter estimation results.

2. THEORY

2.1. Water Flow

In our analysis of the tension disc infiltrometer data we will use a numerical solution of the Richards' equation coupled with the Levenberg-Marquardt nonlinear minimization method [*Marquardt*, 1963]. The governing flow equation for radially symmetric isothermal Darcian flow in a variably-saturated isotropic rigid porous medium is given by the following modified form of the Richards' equation:

$$\frac{\partial \theta}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\, K\, \frac{\partial h}{\partial r} \right) + \frac{\partial}{\partial z}\left(K\, \frac{\partial h}{\partial z} \right) - \frac{\partial K}{\partial z} \tag{1}$$

where θ is the volumetric water content [$L^3 L^{-3}$], h is the pressure head [L], K is the hydraulic conductivity [LT^{-1}], r is a radial coordinate [L], z is the vertical coordinate [L] positive downward, and t is time [T]. Equation (1) is solved numerically for the following initial and boundary conditions applicable to a disc tension infiltrometer experiment:

$$\begin{aligned}
\theta(r,z,t) &= \theta_i(z) & t &= 0 \\
h(r,z,t) &= h_i(z) & t &= 0
\end{aligned} \tag{2}$$

$$h(r,z,t) = h_0(t) \qquad 0 < r < r_0\ , z = 0 \tag{3}$$

$$\frac{\partial h(r,z,t)}{\partial z} = 1 \qquad r > r_0\ , z = 0 \tag{4}$$

$$h(r,z,t) = h_i \qquad r^2 + z^2 \rightarrow \infty \tag{5}$$

5

where θ_i is the initial water content [$L^3 L^{-3}$], h_i is the initial pressure head [L], h_0 is the time-variable supply pressure head imposed by the tension disc infiltrometer [L], and r_0 is the disc radius [L]. Equation (2) specifies the initial condition in terms of either the water content or the pressure head. Boundary condition (3) prescribes the time-variable pressure head under the tension disc permeameter, while (4) assumes a zero flux at the remainder of the soil surface (evaporation is neglected during the short-duration infiltration experiments). Equation (5) states that the other boundaries are sufficiently distant from the infiltration source so that they do not influence the flow process. The boundary condition at the axis of symmetry (r=0) is a no-flow condition. Equation (1), subject to the above initial and boundary conditions, is solved using a quasi three-dimensional (axisymmetric) finite element code, HYDRUS-2D, as documented by *Šimůnek et al.* [1999a].

2.2. Soil Hydraulic Properties

The parameter optimization approach requires the selection of a certain parametric model of the unsaturated soil hydraulic properties prior to application of the numerical solution of the Richards' equation. In this study we will limit ourselves to the unsaturated soil hydraulic functions of *van Genuchten* [1980]:

$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_S - \theta_r} = \frac{1}{(1 + | \alpha h |^n)^m} \tag{6}$$

$$K(\theta) = K_S S_e^l [1 - (1 - S_e^{1/m})^m]^2 \tag{7}$$

where S_e is the effective fluid saturation [-], K_s is the saturated hydraulic conductivity [LT^{-1}], θ_r and θ_s denote the residual and saturated water contents [$L^3 L^{-3}$], respectively; l is the pore-connectivity parameter [-], and α [L^{-1}], n [-], and m (= 1 - 1/n) [-] are empirical shape parameters. The pore-connectivity parameter l in $K(\theta)$ was estimated by *Mualem* [1976] to be 0.5 as an average for many soils. Taking l=0.5, the above hydraulic functions contain 5 unknown parameters: θ_r, θ_s, α, n, and K_s. We will refer to equations (6) and (7) as the van Genuchten - Mualem (VGM) model.

2.3. Formulation of the Inverse Problem

The objective function Φ to be minimized during the parameter estimation process can be formulated in terms of an arbitrary combination of cumulative infiltration data, TDR-measured water contents, and/or tensiometer (pressure head) readings. The objective function is defined as [*Šimůnek and van Genuchten*, 1996]

$$\Phi(\boldsymbol{\beta}, \mathbf{q}_m) = \sum_{j=1}^{m} \left(v_j \sum_{i=1}^{n_j} w_{ij} [q_j^*(t_i) - q_j(t_i, \boldsymbol{\beta})]^2 \right) \tag{8}$$

where m represents different sets of measurements (e.g., infiltration data, the final water content); n_j is the number of measurements in a particular set, $q_j^*(t_i)$ is the specific measurement at time t_i for the jth measurement set, $\boldsymbol{\beta}$ is the vector of optimized parameters (e.g., θ_r, θ_s, α, n, K_s, and l), $q_j(t_i, \boldsymbol{\beta})$ represents the corresponding model predictions for parameter vector $\boldsymbol{\beta}$, and v_j and w_{ij} are weights associated with a particular measurement set j or a measurement i within set j, respectively. We assume that the weighting coefficients w_{ij} in (8) are equal to one, that is, the variances of the errors inside a particular measurement set are all the same. The weighting coefficients v_j are given by

$$v_j = \frac{1}{n_j \, \sigma_j^2} \tag{9}$$

The above approach views the objective function as the average weighted squared deviation normalized by measurement variances σ_j^2. Minimization of the objective function Φ is accomplished by using the Levenberg-Marquardt nonlinear minimization method [*Marquardt*, 1963; *Bard*, 1974].

3. EXAMPLES

3.1. Riverside Example

The numerical inversion method was applied to tension disc infiltrometer data obtained in two field studies. In the first study [*Šimůnek et al.*, 1998b], two tension disc experiments were carried out on a fine sandy loam in Riverside, California. The tension disc had a diameter of 20 cm, while the experiment was executed with three consecutive tensions of 20, 10, and 3 cm. Each tension was maintained for about one hour. Pressure transducers were used to record transient infiltration rates in a setup similar to that described by *Ankeny et al.* [1988]. The soil hydraulic properties were also independently measured with standard laboratory methods on five soil samples. Figure 1 shows the experimental and fitted cumulative infiltration curves versus time for the two runs. The soil hydraulic parameters determined by parameter estimation and with Wooding's analysis are given in Table 1. Unsaturated hydraulic conductivities obtained by parameter estimation corresponded closely with those obtained with Wooding's analysis. For the first experimental run the differences in *K* were only 8.8 and 27% at pressure heads of -6.5 and -15 cm, respectively. The two sets of unsaturated hydraulic conductivities differed by only about 30% for the second experiment. The differences were higher for the extrapolated values of K_s (34 and 47%), but even those differences appear acceptable for most practical applications.

Excellent agreement between the measured and fitted cumulative field infiltration curves was obtained when the five main soil hydraulic parameters in van Genuchten's model were optimized (Figure 1). Hydraulic conductivities (both saturated and unsaturated) as determined by the numerical inversion compared well with those obtained using Wooding's analytical solution (Table 1). Agreement between retention curves obtained by numerical inversion of the field infiltration experiment and by direct laboratory measurement, however, was relatively poor. The entire laboratory retention curve shifted by about 0.10 units towards higher water contents, while also the parameter *n* had different values (α-values were much closer for both analyses). The infiltration experiment could not be closely reproduced when the mean laboratory soil hydraulic parameters were used and the closed-form van Genuchten-Mualem model was assumed to be valid [*Šimůnek et al.*, 1998b].

Table 1. Comparison of results obtained with Wooding's analysis and using parameter estimation.

Parameter	Run 1			Run 2		
	Wooding's Analysis		Parameter Est.	Wooding's Analysis		Parameter Est.
	(-10,-20 cm)	(-3,-10 cm)		(-10,-20 cm)	(-3,-10 cm)	
α (cm^{-1})			0.0412			0.0406
n (-)			3.61			2.76
θ_s (m^{3}m^{-3})			0.274			0.238
K_s (cm d^{-1})	32.03	14.00	9.24 (-34.1%)*	20.42	12.33	6.57 (-46.72%)
K(-6.5cm) (cm d^{-1})		9.65	8.80 (-8.81%)		7.26	5.34 (-26.44%)
K(-15cm) (cm d^{-1})	6.81		4.95 (-27.31%)	3.74		2.49 (-33.42%)
α^*(-6.5cm) (cm^{-1})		0.0572			0.113	
α^*(-15cm) (cm^{-1})	0.103			0.0814		

[*] The number in parentheses shows by how many percent the hydraulic conductivity obtained by parameter estimation differs from corresponding values obtained using Wooding's analysis.
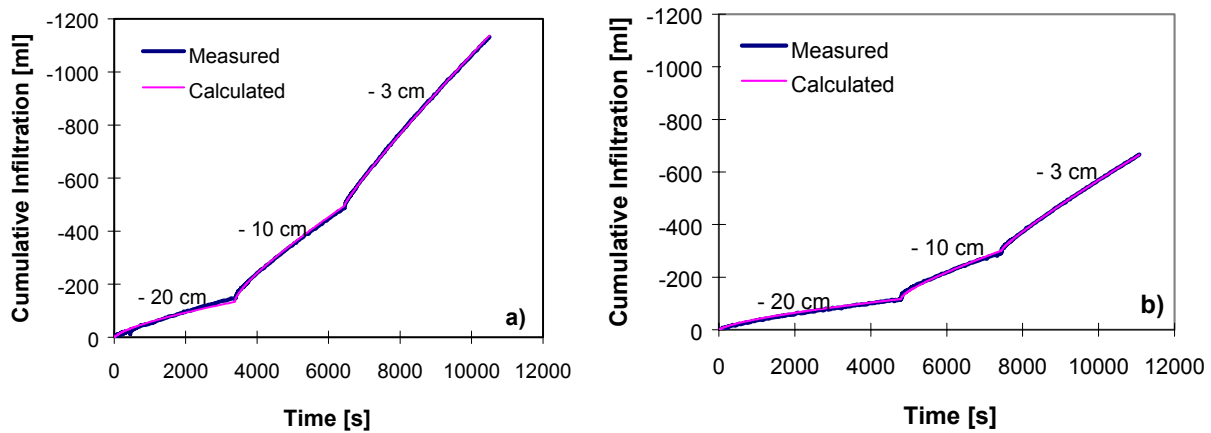

Fig. 1. Measured and fitted cumulative infiltration curves versus time for the a) first and b) second infiltration experiment.

3.2. Sahel Example

In this example [*Šimůnek et al.,* 1998a] we use numerical inversion to estimate the hydraulic properties of a two-layered crusted soil system in the Sahel region of Africa. Here we will report only results for the sandy subsoil obtained with a tension disc diameter of 25 cm and for supply tensions of 11.5, 9, 6, 3, 1, and 0.1 cm. Figure 2 shows measured and optimized cumulative infiltration curves. The small breaks in the infiltration curve were caused by brief interruptions to resupply the infiltrometer with water, and to adjust the tension for a new time interval. Very close agreement between the measured and optimized cumulative infiltration curves was obtained; the largest deviations were generally less than 60 ml, which was only about 0.5% of the total infiltration volume. Figure 3 compares the parameter estimation results against results obtained with Wooding's analysis. Both methods gave almost identical unsaturated hydraulic conductivities for pressure heads in the interval between -2 and -10.25 cm. However, the hydraulic conductivity obtained with Wooding's analysis at the highest pressure head overestimated the inverse results by a factor of two. *Šimůnek et al.* [1998a] further compared the numerical inversion results with hydraulic properties estimated from available soil textural information using the neural-network-based pedotransfer functions of *Schaap et al.* [1998]. Relatively good agreement between the inverse and neural network predictions was obtained (results not further shown here). Additional applications of inverse modeling to transient tension disc infiltration experiments are given by *Šimůnek et al.* [1999b].
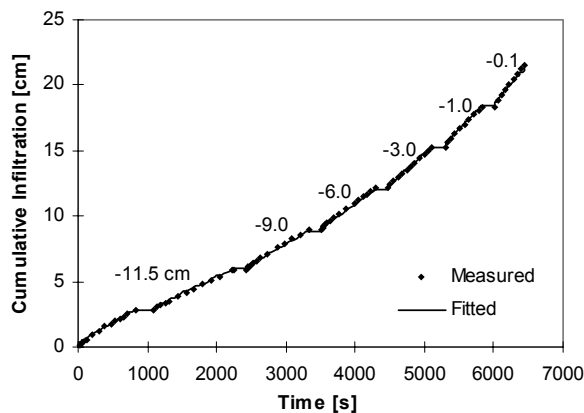

Figure 3. Measured and optimized cumulative infiltration curves for a tension disc infiltrometer experiment carried out on a sandy soil in the Sahel region.
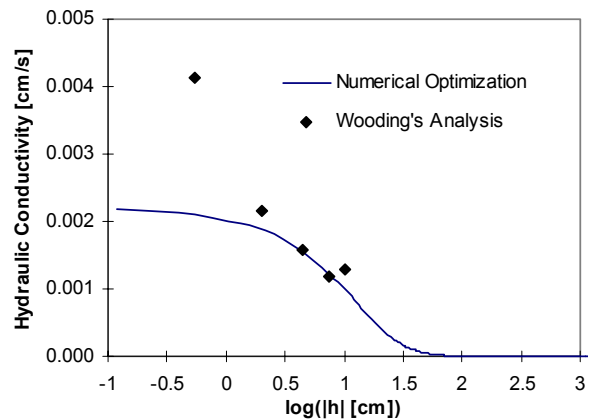
Figure 4. Unsaturated hydraulic conductivities calculated using Wooding's analytical solution, and the complete function obtained with numerical inversion.

11

4. DESCRIPTION OF INPUT FILES

The input information is organized into one file DISC.IN. This input file is generated with the help of a Windows graphical interface that uses the entered information. Several additional input files (MESHTRIA.001 and BOUNDARY.001 through MESHTRIA.003 and BOUNDARY.003), which give information about the relative finite element nodal distribution and the boundary conditions, are located in subdirectory DISKDATA and were pregenerated. From the information given in these files the finite element mesh is scaled to the actual geometry.

Table 2. Input File DISC.IN - Inverse Solution Information.

_____

Record	Type	Variable	Description
1	Char	*Title*	Descriptive title for simulation.
2	-	-	Comment line.
3	Integer	*NOBB*	Number of observed data (cumulative infiltration versus time).
3	Integer	*MIT*	Maximum number of iterations for the inverse problem (recommended value is 50).
3	Integer	*NofBC*	Number of time-variable values in the disc boundary condition.
4	-	-	Comment line.
5	Char	*LUnit*	Length units (e.g., mm, cm, m)
6	Char	*TUnit*	Time units (e.g., sec, min, hours, days)
7	-	-	Comment line.
8	Real	*tInit*	Initial (starting) time [T].
8	Real	*dtInit*	Initial time step [T], recommended value is about 1 s.
8	Real	*dtMin*	Minimum allowed time step [T], recommended value is about 0.01 s.
9	-	-	Comment line.
10	Integer	*Mesh*	Type of finite element mesh used for simulation. =1: Very fine mesh with 2145 triangular elements (slow and stable solution. =2: Fine mesh with 1611 triangular elements. =3: Course mesh with 1073 triangular elements (faster solution, but may result in unstable solution).
10	Real	*ThetaI*	Initial water content under the tension disc infiltrometer.
10	Real	*ThetaF*	Final water content directly under the tension disc infiltrometer. This value corresponds with the final supply pressure head of the disc.
10	Real	*DiskR*	Disk radius [L].
11	-	-	Comment line.
12	Real	*Par*(1,*M*)	Initial estimate of parameter θ_r for material M [-].
12	Real	*Par*(2,*M*)	Initial estimate of parameter θ_s for material M [-].
12	Real	*Par*(3,*M*)	Initial estimate of parameter α for material M [L^{-1}].
12	Real	*Par*(4,*M*)	Initial estimate of parameter n for material M [-].
12	Real	*Par*(5,*M*)	Initial estimate of parameter K_s for material M [LT^{-1}].
12	Real	*Par*(6,*M*)	Initial estimate of parameter l for material M [-].
13	Integer	*Index*(1,*M*)	Parameter estimation index for parameter θ_r, material M [-]. = 0; Coefficient is known and kept constant during optimization. = 1; Coefficient is unknown and estimated by curve fitting the data.
13	Integer	*Index*(2,*M*)	Parameter estimation index for parameter θ_s, material M [-].
13	Integer	*Index*(3,*M*)	Parameter estimation index for parameter α, material M [-].
13	Integer	*Index*(4,*M*)	Parameter estimation index for parameter n, material M [-].

Record	Type	Variable	Description
13	Integer	$Index(5,M)$	Parameter estimation index for parameter K_s, material M [-].
13	Integer	$Index(6,M)$	Parameter estimation index for parameter l, material M [-].
14	Real	$BMn(1,M)$	Minimum constraint for parameter θ_r for material M [-] (dummy value if $Index(1,M)$=0).
14	Real	$BMn(2,M)$	Minimum constraint for parameter θ_s, material M [-].
14	Real	$BMn(3,M)$	Minimum constraint for parameter α, material M [L^{-1}].
14	Real	$BMn(4,M)$	Minimum constraint for parameter n, material M [-].
14	Real	$BMn(5,M)$	Minimum constraint for parameter K_s, material M [LT^{-1}].
14	Real	$BMn(6,M)$	Minimum constraint for parameter l, material M [-].
15	Real	$BMx(1,M)$	Maximum constraint for parameter θ_r, material M [-] (dummy value if $Index(1,M)$=0).
15	Real	$BMx(2,M)$	Maximum constraint for parameter θ_s, material M [-].
15	Real	$BMx(3,M)$	Maximum constraint for parameter α, material M [L^{-1}].
15	Real	$BMx(4,M)$	Maximum constraint for parameter n, material M [-].
15	Real	$BMx(5,M)$	Maximum constraint for parameter K_s, material M [LT^{-1}].
15	Real	$BMx(6,M)$	Maximum constraint for parameter l, material M [-].
16	-	-	Comment line.
17	Real	$Time(i)$	Time t for the first boundary condition.
17	Real	$hBound(i)$	Pressure head h applied with the tension disc infiltrometer [L]. A value of 99 represents a zero flux BC. This boundary condition is used when the disc is removed to resupply it with water. Record 17 is provided $NofBC$ times.
18	-	-	Comment line.
19	Real	$HO(i)$	Observation data. Time t.
19	Real	$FO(i)$	Observation data. Cumulative infiltration I. Record 19 is provided $NOBB$ times.

Table 3. Example of the Input File FIT.IN for the Sahel experiment.

```
Tension Permeameter - Rafael Angulo - Sahel Data
   NOBB      MIT    NofBC
    222       50        13
   LUnits    TUnits
cm
sec
  tInit   dtInit    dtMin
      0        1     0.01
  Mesh   ThetaI   ThetaF   DiskD
     1    0.149    0.275    12.5
   thr       ths     Alfa        n         Ks         l
  0.01      0.28     0.07      1.9      0.003       0.5
      0         1        1        1          1         0
      0      0.27        0      1.1     1e-006        0
      0       0.5        0      4.5        0.7        0
  Time   hBound
   840    -11.5
  1080       99
  2250    -11.5
  2430       99
  3330       -9
  3510       99
  4290       -6
  4470       99
  5115       -3
  5295       99
  5835       -1
  6015       99
  6450     -0.1
  HO(N)         FOS
    15       44.3486
    30        90.809
    45       137.269
    60       173.171
    75       209.072
    90       238.638
     -           -
     -           -
  6390      10370.2
  6405      10414.5
  6435      10509.6
  6450      10562.4
end*** END OF INPUT FILE 'FIT.IN' ************************
```

16

5. DESCRIPTION OF THE OUTPUT FILE

Results of the inverse solution are directed into an output file FIT.OUT. As part of the inverse solution, DISC produces a correlation matrix that specifies the degree of correlation between the fitted coefficients. The correlation matrix quantifies changes in model predictions caused by small changes in the final estimate of a particular parameter, relative to similar changes as a result of changes in the other parameters. The correlation matrix reflects the nonorthogonality between two parameter values. A value of ±1 reflects perfect linear correlation whereas 0 indicates no correlation at all. The correlation matrix may be used to select which parameters, if any, are best kept constant in the parameter estimation process because of high correlation.

An important measure of the goodness of fit is the r^2 value for regression of the observed, $\hat{y}_i$, versus fitted, $y_i(\boldsymbol{\beta})$, values:

$$r^2 = \frac{\left[\sum w_i \hat{y}_i y_i - \dfrac{\sum \hat{y}_i \sum y_i}{\sum w_i}\right]^2}{\left[\sum w_i \hat{y}_i^2 - \dfrac{\left(\sum \hat{y}_i\right)^2}{\sum w_i}\right]\left[\sum y_i^2 - \dfrac{\left(\sum y_i\right)^2}{\sum w_i}\right]} \qquad (10)$$

The r^2 value is a measure of the relative magnitude of the total sum of squares associated with the fitted equation; a value of 1 indicates a perfect correlation between the fitted and observed values.

DISC provides additional statistical information about the fitted parameters such as the mean, standard error, T-value, and the lower and upper confidence limits (given in output file FIT.OUT). The standard error, $s(\beta_j)$, is estimated from knowledge of the objective function, the number of observations, the number of unknown parameters to be fitted, and an inverse matrix [*Daniel and Wood*, 1971]. The T-value is obtained from the mean and standard error using the equation

$$T = \frac{\beta_j}{s(\beta_j)} \qquad (11)$$

The values for T and $s(\beta_j)$ provide absolute and relative measures of the deviations around the mean. DISC also specifies the upper and lower bounds of the 95% confidence level around each fitted parameter β_j. It is desirable that the real value of the target parameter always be located in a narrow interval around the estimated mean as obtained with the optimization program. Large confidence limits indicate that the results are not very sensitive to the value of a particular parameter.

Finally, because of possible problems related to convergence and parameter uniqueness, we recommend to routinely rerun the program with different initial parameter estimates to verify that the program indeed converges to the same global minimum in the objective function. This is especially important for field data sets which often exhibit considerable scatter in the measurements, or may cover only a narrow range of soil water contents and pressure heads. Whereas DISC will not accept initial estimates that are out of range, it is ultimately the user's responsibility to select meaningful initial estimates. One recommended way of doing this is to use pedotransfer functions. This may be especially advantageous if little or no information is available to define the dry sides of the water retention and hydraulic curves. In this case one could even predict the residual water content, θ_r, with pedotransfer functions and subsequently keep θ_r constant during the optimization process. The DISC software contains pedotransfer functions [*Schaap et al.,* 1998] that could be used immediately for this purpose.

Table 4. FIT.OUT - parameter estimation related information.

_____

SSQ	Value of the objective function Φ being minimized during the parameter optimization process.
S.E.Coeff	Standard error.
RSQUARE	r^2 value for regression of observed versus fitted values.
Quantity	Measured data, e.g., the pressure head, water content, cumulative flux.
Type	Type of measured data (corresponds to Table 10.10 of the HYDRUS-1D manual).
Position	Position of the measurement (corresponds to Table 10.10 of the HYDRUS-1D manual).
Weight	Weight associated with a particular data point.
Residual	Residual between measured and fitted quantity.

_____

6. USERS MANUAL

The computational module of the DISC software package (DISKTENS) is written in FORTRAN. However, the interactive graphics-based interface for the MS Windows environment was written in C++. In addition to information given in this chapter, extensive context-sensitive on-line help is made part of the interface. By pushing the F1 button, or clicking on the Help button while working in any window, the user obtains information about the window content. In addition, context-sensitive help is available using the "SHIFT+F1" help button. In this mode the mouse cursor changes to a help cursor (a combination of arrow + question mark), and the user can proceed by clicking on the object for which help is needed (i.e., a menu item, toolbar button, or other feature). At this point a help file will be displayed, giving information about the item on which the user clicked.

DISC is the main program unit defining the overall computational environment of the system. This module controls execution of the program and determines which other optional modules are necessary for a particular application. The module contains a project manager and both the pre-processing and post-processing units. The pre-processing unit includes specification of all necessary parameters to successfully run the FORTRAN codes. The post-processing unit consists of simple x-y plots for graphical presentation of the results and a dialog window that displays an ASCII output file.

The work for a new project should begin by opening the **Project Manager**, and giving a name and brief description of the new project. Users must also decide where to save the project's data (to which workspace). Then select the Type of Problem command from the Input Menu. From this point on the program will navigate the user through the entire process of entering input data. The user may either select particular commands from a menu, or allow the interface to lead him/her through the process of entering input data by repeatedly selecting the Next button. Alternatively, clicking the Previous button will return the user to the previous window.

The **Project Manager** is used to manage data of existing projects, and to help locate, open, copy, delete and/or rename desired projects or their input or output data. A "project" represents any particular problem to be solved by DISC. The project name (8 letters maximum), as well as a brief description of the project, helps to locate a particular problem. Input and output

data for each project are placed in a subdirectory with the same name as the project. Projects are represented by a file *project_name.dsc* and the *project_name* subdirectory.

   The **Project Manager** gives users considerable freedom in terms of organizing his/her projects. The projects are grouped into **Workspaces** that can be placed anywhere in accessible memory, i.e., on local and/or network hard drives. The **Workspace** can be any existing accessible subdirectory (folder). DISC is installed together with a default workspace with three examples described in Chapter 4. We suggest that the user creates his/her own workspaces, e.g., the *MyTests* workspace, and keeps the provided examples intact for further reference. Projects can be copied with the **Project Manager** only within a particular workspace. Users can copy projects between workspaces using standard file managing software, e.g., Windows Explorer. In that case users must copy both the subdirectory of a particular project and the *project_name.dsc* file. Another way of copying a project between Workspaces is to first open the project and then using the command <u>Save as</u> to save this project to a new location.

7. REFERENCES

Ankeny, M. D., M. Ahmed, T. C. Kaspar, and R. Horton, Simple field method for determining unsaturated hydraulic conductivity, *Soil Sci. Soc. Am. J., 55*, 467-470, 1991.

Bard, Y., Nonlinear parameter estimation, Academic Press, New York, N.Y., 341pp., 1974.

Bohne, K., C. Roth, F. J. Leij, and M. Th. van Genuchten, Rapid method for estimating the unsaturated hydraulic conductivity from infiltration measurement, *Soil Sci., 155*(4), 237-244, 1992.

Bruce, R. R., and A. Klute, The measurement of soil moisture diffusivity, *Soil Sci. Soc. Am. Proc., 20*, 458-462, 1956.

Celia, M. A., and E. T. Bouloutas, R. L. Zarba, A general mass-conservative numerical solution for the unsaturated flow equation, *Water Resour. Res., 26*(7), 1483-1496, 1990.

Cuenca, R. H., Brouwer, J., Chanzy, A., Droogers, P., Galle, S., Gaze, S. R., Sicot, M., Stricker, H., Angulo-Jaramillo, R., Boyle, S. A., Bromly, J. Chebhouni, A. G., Cooper, J. D., Dixon, A. J., Fies, J.-C., Gandah, M., Gaudu, J.-C., Laguerre, L., Soet, M., Steward, H. J., Vandervaere, J.-P., Vauclin, M., Soil measurements during HAPEX-Sahel intensive observation period, *J. of Hydrol., 188-189*, 224-266, 1997.

Dane, J. H. and S. Hruska, In-situ determination of soil hydraulic properties during drainage, *Soil Sci. Soc. Am. J., 47*, 619-624, 1983.

Daniel, C., and F. S. Wood. 1971. *Fitting Equations to Data*. Wiley-Interscience, New York.

Eching, S. O., J. W. Hopmans, and O. Wendroth, Optimization of hydraulic functions from transient outflow and soil water pressure data, *Soil Sci. Soc. Am. J., 57*, 1167-1175, 1993.

Gardner, W. R., Some steady-state solutions of the unsaturated moisture flow equation with application to evaporation from a water table, *Soil Sci., 85*, 228-232, 1958.

Green, R. E., L. R. Ahuja, and S. K. Chong, Hydraulic conductivity, diffusivity, and sorptivity of unsaturated soils: field methods, in A. Klute (ed.), *Methods of Soil Analysis*, Part 1. 2nd ed., Agronomy Monogr. 9, ASA and SSSA, Madison, WI, pp. 771-798, 1986.

Klute, A. and C. Dirksen, Hydraulic conductivity and diffusivity: Laboratory methods, in A. Klute (ed.), *Methods of Soil Analysis*, Part 1. 2nd ed., Agronomy Monogr. 9, ASA and SSSA, Madison, WI, pp. 687-734, 1986.

Kool, J. B., J. C. Parker, and M. Th. van Genuchten, ONESTEP: A nonlinear parameter estimation program for evaluating soil hydraulic properties from one-step outflow experiments, *Virginia Agric. Exp. Stat. Bull.* 85-3, Blacksburg, VA, 1985a.

Kool, J. B., J. C. Parker, and M. Th. van Genuchten, Determining soil hydraulic properties from one-step outflow experiments by parameter estimation: I. Theory and numerical studies, *Soil Sci. Soc. Am. J., 49*, 1348-1354, 1985b.

Kool, J. B., J. C. Parker, and M. Th. van Genuchten, Parameter estimation for unsaturated flow and transport models - A review, *J. Hydrol., 91*, 255-293, 1987.

Kool, J. B., and J. C. Parker, Analysis of the inverse problem for transient unsaturated flow, *Water Resour. Res., 24*(6), 817-830, 1988.

Logsdon, S. D., E. L. McCoy, R. R. Allmaras, and D. R. Linden, Macropore characterization by indirect methods, *Soil Sci., 155*, 316-324, 1993.

Marquardt, D. W., An algorithm for least-squares estimation of nonlinear parameters, *SIAM J. Appl. Math., 11*, 431-441, 1963.

Mualem, Y., A new model for predicting the hydraulic conductivity of unsaturated porous media, *Water Resour. Res. 12*, 513-522, 1976.

Parker, J. C. and M. Th. van Genuchten, Determining transport parameters from laboratory and field tracer experiments, *Bull*. 84-3, Va. Agric. Exp. Stat., Blacksburg, VA, 96 pp., 1984.

Parker, J. C., J. B. Kool, and M. Th. van Genuchten, Determining soil hydraulic properties from one-step outflow experiments by parameter estimation: II. Experimental studies, *Soil Sci. Soc. Am. J., 49*, 1354-1359, 1985.

Perroux, K. M., and I. White, Design for disc permeameters, *Soil Sci. Soc. Am. J., 52*, 1205-1215, 1988.

Reynolds, W. D., and D. E. Elrick, Determination of hydraulic conductivity using a tension infiltrometer, *Soil Sci. Soc. Am. J., 55*, 633-639, 1991.

Russo, D., E. Bresler, U. Shani, and J. C. Parker, Analysis of infiltration events in relation to determining soil hydraulic properties by inverse problem methodology, *Water Resour. Res., 27*(6), 1361-1373, 1991.

Schaap, M. G., Leij F. J. and van Genuchten M. Th., Neural network analysis for hierarchical prediction of soil water retention and saturated hydraulic conductivity, *Soil Sci. Soc. Am. J.*, 62, 847-855, 1998.

Šimůnek, J., and M. Th. van Genuchten, Estimating unsaturated soil hydraulic properties from tension disc infiltrometer data by numerical inversion, *Water Resour. Res., 32*(9), 2683-2696, 1996.

Šimůnek, J., and M. Th. van Genuchten, Estimating unsaturated soil hydraulic properties from multiple tension disc infiltrometer data, *Soil Science, 162*(6), 383-398, 1997.

Šimůnek, J., R. Angulo-Jaramillo, M. G. Schaap, J.-P. Vandervaere, and M. Th. van Genuchten, Using an inverse method to estimate the hydraulic properties of crusted soils from tension disc infiltrometer data, *Geoderma, 86*, 61-81, 1998a.

Šimůnek, J., D. Wang, P. J. Shouse, and M. Th. van Genuchten, Analysis of a field tension disc infiltrometer experiment by parameter estimation, *Intern. Agrophysics, 12*, 167-180, 1998b.

Šimůnek, J., M. Šejna, and M. Th. van Genuchten, The HYDRUS-2D software package for simulating two-dimensional movement of water, heat, and multiple solutes in variably saturated media. Version 2.0, *IGWMC - TPS - 53,* International Ground Water Modeling Center, Colorado School of Mines, Golden, Colorado, 251pp., 1999a.

Šimůnek, J., O. Wendroth, and M. Th. van Genuchten, Estimating unsaturated soil hydraulic properties from laboratory tension disc infiltrometer experiments, *Water Resour. Res., 35*(10), 2965-2979, 1999b.

Smettem, K. R. J., and B. E. Clothier, Measuring unsaturated sorptivity and hydraulic conductivity using multiple disk permeameters, *J. Soil Science, 40*, 563-568, 1989.

van Dam, J. C., J. N. M. Stricker, and P. Droogers, Inverse method for determining soil hydraulic functions from one-step outflow experiment, *Soil Sci. Soc. Am. Proc., 56*, 1042-1050, 1992.

van Dam, J. C., J. N. M. Stricker, and P. Droogers, Inverse method to determine soil hydraulic functions from multistep outflow experiment, *Soil Sci. Soc. Am. Proc., 58*, 647-652, 1994.

van Genuchten, M. Th., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Soc. Am. J., 44*, 892-898, 1980.

van Genuchten, M. Th., Non-equilibrium transport parameters from miscible displacement experiments, *Research Report No.* 119, U. S. Salinity Laboratory, USDA, ARS, Riverside, CA, 1981.

van Genuchten, M. Th., and F. J. Leij, On estimating the hydraulic properties of unsaturated soils, In: M. Th. van Genuchten, F. J. Leij and L. J. Lund (eds.), Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils, pp. 1-14, Univ. of California, Riverside, 1992.

van Genuchten, M. Th., and J. Šimůnek, Evaluation of pollutant transport in the unsaturated zone, *Proc. Regional Approaches to Water Pollution in the Environment*, NATO Advanced Research Workshop, Liblice, Czech Republic (in press), 1995.

White, I., and M. J. Sully, Macroscopic and microscopic capillary length and time scales from field infiltration, *Water Resour. Res., 23*, 1514-1522, 1987.

Wooding, R. A., Steady infiltration from large shallow circular pond, *Water Resour. Res., 4*, 1259-1273, 1968.

Zachmann, D. W., P. C. Duchateau, and A. Klute, Simultaneous approximation of water capacity and soil hydraulic conductivity by parameter identification, *Soil Sci., 134*, 157-163, 1981.