AUTOMATIC ANALYSIS OF MULTIPLE BEERKAN INFILTRATION EXPERIMENTS FOR SOIL HYDRAULIC CHARACTERIZATION

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Abstract: The BEST (Beerkan Estimation of Soil Transfer parameters) procedure of soil hydraulic characterization appears promising for intensively sampling field areas with a reasonable effort in terms of both equipment and time passed in the field. Alternative algorithms have been suggested to determine soil sorptivity and saturated soil hydraulic conductivity from a simply measured cumulative infiltration curve. With these algorithms, calculations have to be repeated several times, depending on the number of collected infiltration data, that should vary between eight and 15. The need to consider a variable number of infiltration data is related to the fact that the infiltration model used in BEST is valid for the transient phase of the process, and only experimental data representative of this phase of the infiltration process have to be selected. The fitting of the theoretical model to the data is carried out by minimizing the sum of the squared residuals between model-predicted and measured infiltration data. Therefore, analyzing a single run may demand a lot of time, since many calculations have to be carried out. This circumstance complicates soil hydraulic characterization based on an intensive soil sampling, and it also increases the risk to make mistakes. These problems are expected to be substantially reduced, or even eliminated, if an automatic procedure of data analysis is applied. The general objective of this investigation was to develop a workbook to easily and rapidly analyze databases including several BEST runs. The developed workbook makes use of the Microsoft Excel Solver add-in routine. A Visual Basic for Applications (VBA) macro was written to automate creation and manipulation of Microsoft Excel Solver. A looping structure was used in the VBA macro to automate data analysis of BEST experiments. The workbook can be viewed as a practically useful contribution to an expeditious, intensive soil hydraulic characterization, also in terms of analysis of the collected data.

Key words: Soil hydraulic properties, Measurement methods, BEST (Beerkan Estimation of Soil Transfer parameters) procedure, Automatic data processing tool

1. INTRODUCTION

Interpreting and modeling soil hydrological processes require the determination of the soil hydraulic characteristic curves, i.e. the relationships between volumetric soil water content, soil water pressure head, and soil hydraulic conductivity. Using traditional methods to determine these properties is expensive and time consuming. Haverkamp et al. (1996) pioneered a specific method for soil hydraulic characterization known as the "Beerkan method". An improved version of this methodology, called the Beerkan Estimation of Soil Transfer parameters (BEST) procedure, was developed by Lassabatère et al. (2006) to simplify soil hydraulic characterization. BEST considers certain analytic formulae for hydraulic characteristic curves and estimates their shape parameters, which are texture dependent, from particle-size analysis by physical-empirical pedotransfer functions. Structure dependent scale parameters are estimated by a three-dimensional (3D) field infiltration experiment at zero pressure head, using the two-term transient infiltration equation by Haverkamp et al. (1994).

According to Yilmaz et al. (2010), the original algorithm to analyze the infiltration data, named BEST-slope, may lead to erroneous values of saturated soil hydraulic conductivity, K_s, especially when a very high level of precision relative to the steady-state infiltration rate cannot be obtained. These authors introduced a revised version of BEST (BEST-intercept) to avoid obtaining negative K_s values. Differences by a factor of more than an order of magnitude were reported by Yilmaz et al. (2010) for the K_s values of basic oxygen furnace slag obtained with the two algorithms. The conclusion by these Authors was that BEST-intercept yielded a more reliable soil hydraulic characterization than BEST-slope.

Bagarello et al. (2013) proposed a third alternative algorithm (BEST-steady) making exclusive use of the steady-state phase of the infiltration run. The expected advantage of BEST-steady algorithm is that the possible problems associated with the use of the transient infiltration data are avoided.

The general objective of this investigation was to develop a workbook to easily and rapidly analyze databases including several BEST runs. The developed workbook makes use of the Microsoft Excel Solver add-in routine. A Visual Basic for Applications (VBA) macro was written to automate creation and manipulation of Microsoft Excel Solver models. A looping structure was used in the VBA macro to automate data analysis of BEST experiments.

2. THEORY

2.1 Beerkan Estimation of Soil Transfer parameters (BEST) procedure

The BEST procedure for soil hydraulic characterization (Lassabatère et al., 2006) focuses specifically on the van Genuchten (1980) relationship for the water retention curve with the Burdine (1953) condition and the Brooks and Corey (1964) relationship for hydraulic conductivity:

$$\frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[1 + \left(\frac{h}{h_g}\right)^n\right]^{-m} \tag{1a}$$

$$m = 1 - \frac{2}{n} \tag{1b}$$

$$\frac{K(\theta)}{K_s} = \left(\frac{\theta - \theta_r}{\theta_s - \theta_r}\right)^{\eta} \tag{2a}$$

$$\eta = \frac{2}{m \times n} + 3 \tag{2b}$$

where θ (L^3L^{-3}) is the volumetric soil water content, h (L) is the soil water pressure head, K ($L\ T^{-1}$) is the soil hydraulic conductivity, n, m and η are shape parameters, and h_g (L), θ_s (L^3L^{-3}, saturated soil water content), θ_r (L^3L^{-3}, residual soil water content) and K_s ($L\ T^{-1}$, saturated soil hydraulic conductivity) are scale parameters. In the BEST procedure, θ_r is assumed to be zero. Estimation of n is based on the soil particle size distribution (PSD), which is modeled as:

$$P(D) = \left[1 + \left(\frac{D_g}{D}\right)^N\right]^{-M} \tag{3}$$

where $P(D)$ is the fraction by mass of particles passing a particular diameter, D (L), D_g (L) is a scale parameter, and N and $M = 1 - 2/N$ are shape factors. Fitting eq.(3) to the measured PSD allows to calculate the shape index for PSD, p_M:

$$p_M = \frac{MN}{1 + M} \tag{4}$$

The m parameter of eq.(1) is calculated by:

$$m = \frac{1}{p_m}\left(\sqrt{1 + p_m^2} - 1\right) \tag{5}$$

2

where:

$$p_m = p_M(1+\kappa)^{-1} \tag{6}$$

$$\kappa = \frac{2s-1}{2s(1-s)} \tag{7}$$

$$(1-f)^s + f^{2s} = 1 \tag{8}$$

where f (L³L⁻³) is the soil porosity and s is the fractal dimension of the media, varying from 0.5 to 1 (Minasny and McBratney, 2007).

An alternative way to estimate the n parameter used with the BEST procedure from the soil sand, sa (%, USDA classification), and clay, cl (%), content was proposed by Minasny and McBratney (2007):

$$n = 2.18 + 0.11[48.087 - 44.954S(x_1) - 1.023S(x_2) - 3.896(x_3)] \tag{9a}$$

Where:

$$x_1 = 24.547 - 0.238 \ sa - 0.082 \ cl \tag{9b}$$

$$x_2 = -3.569 + 0.081 \ sa \tag{9c}$$

$$x_3 = 0.694 - 0.024 \ sa + 0.048 \ cl \tag{9d}$$

$$S(x) = \frac{1}{1+\exp(-x)} \tag{9e}$$

For an infiltration experiment with zero pressure on a circular surface of radius r (L) above a uniform soil with a uniform initial water content (θ_0), the three dimensional cumulative infiltration, I (L), and steady state infiltration rate, i_s (L T⁻¹), can be approximated by the following explicit transient two term relationship and steady state expansion:

$$I(t) = S\sqrt{t} + (A \ S^2 + B \ K_s)t \tag{10}$$

$$i_s = A \ S^2 + K_s \tag{11}$$

where t (T) is the time, S (L T⁻¹ᐟ²) is soil sorptivity, and A (L⁻¹) and B are constants that can be defined for the specific case of a Brooks and Corey (1964) relationship (eq.2a) as:

$$A = \frac{\gamma}{r(\theta_s - \theta_0)} \tag{12}$$

$$B = \frac{2-\beta}{3}\left[1 - \left(\frac{\theta_0}{\theta_s}\right)^\eta\right] + \left(\frac{\theta_0}{\theta_s}\right)^\eta \tag{13}$$

where β and γ are coefficients that are commonly set at 0.6 and 0.75, respectively, for $\theta_0 < 0.25 \ \theta_s$ (Smettem et al., 1994; Haverkamp et al., 1994), although a recent investigation suggested that they have a large impact on the estimation procedure (Nasta et al., 2012). Sorptivity can be expressed as a function of the scale parameters by the following relationship:

$$S^2(\theta_0, \theta_s) = -c_p \theta_s K_s h_g \left(1 - \frac{\theta_0}{\theta_s}\right)\left[1 - \left(\frac{\theta_0}{\theta_s}\right)^\eta\right] \qquad (14)$$

where:

$$c_p = \Gamma\left(1 + \frac{1}{n}\right)\left\{\frac{\Gamma\left(m\eta - \frac{1}{n}\right)}{\Gamma(m\eta)} + \frac{\Gamma\left(m\eta + m - \frac{1}{n}\right)}{\Gamma(m\eta + m)}\right\} \qquad (15)$$

where Γ stands for the Gamma function. BEST estimates shape parameters (m, n and η) on the basis of particle size analysis and soil porosity determination whereas the infiltration experiment is used to estimate scale parameters (h_g and K_s). The initial water contents is measured at the beginning of the infiltration experiment. BEST was applied by setting θ_s equal to total soil porosity determined from a bulk density measurement (Mubarak et al., 2009). BEST first estimates sorptivity by fitting the transient cumulative infiltration on eq.(10) with K_s replaced by its sorptivity function and the experimental steady state infiltration rate through eq.(11):

$$K_s = i_s - A S^2 \qquad (16)$$

The fit is performed by minimizing the classical objective functions for cumulative infiltration $I(t)$:

$$f_I(S, K_s, k) = \sum_{i=1}^{k}\left[I^{exp}(t_i) - I(t_i)\right]^2 \qquad (17)$$

where k is the number of considered (t, I) data points for the transient state. Once sorptivity is estimated, K_s is driven through eq.(16), assuming that steady state has been reached. As eq.(10) is valid only at transient state, the fit may not be valid for large values of k. Therefore, BEST fits data for a minimum of five points to a maximum of k_{tot}, i.e. the whole dataset. For each data subset containing the first k points (duration of the experiment equal to t_k), S and K_s are estimated and the time, t_{max} (T), defined as the maximum time for which the transient expressions can be considered valid, is determined:

$$t_{max} = \frac{1}{4(1-B)^2}\left(\frac{S}{K_s}\right)^2 \qquad (18)$$

Then, t_k is compared with t_{max}. The values of S and K_s are not considered valid unless t_k is lower than t_{max}. Among all values of S and K_s that fulfill this condition, the S and K_s values corresponding to the largest k (k_{step}) are retained. The pressure head scale parameter, h_g, is then estimated:

$$h_g = \frac{S^2}{c_p(\theta_s - \theta_0)\left[1 - \left(\frac{\theta_0}{\theta_s}\right)^\eta\right]K_s} \qquad (19)$$

The algorithm described above was named BEST-slope by Yilmaz et al. (2010).

An alternative algorithm, named BEST-intercept, was developed by these last Authors since attempting to estimate K_s by eq.(11) was considered to be inappropriate when i_s approaches AS^2, especially if a very high level of precision relative to the steady state infiltration rate cannot be obtained. More specifically, when the estimated AS^2 value exceeds the infiltration rate at the end of the experiment, the values obtained for K_s are negative. In the new algorithm, Yilmaz et al. (2010) proposed replacing such a constraint by using the intercept ($b_{+\infty}^{end}$) of the asymptotic expansion, $I_{+\infty}(t)$, as defined by the following equation:

$$I_{+\infty}(t) = \left(AS^2 + K_s \right) t + C \frac{S^2}{K_s} \tag{20}$$

where C is equal to:

$$C = \frac{1}{2\left[1 - \left(\dfrac{\theta_0}{\theta_s} \right)^{\eta} \right](1 - \beta)} \ln\left(\frac{1}{\beta} \right) \tag{21}$$

Therefore, the following relationship is applied to determine K_s:

$$K_s = C \frac{S^2}{b_{+\infty}^{end}} \tag{22}$$

This procedure leads to the use of the division operator rather than the subtraction operator and thereby avoids obtaining negative values for the estimation of K_s.

A third algorithm, named BEST-steady, was developed by Bagarello et al. (2013). BEST-steady, makes use of the intercept ($b_{+\infty}^{end}$) and the slope (i_s) of the straight line fitted to the data describing steady-state conditions on the I vs. t plot. Combining equations (16) and (22) yields to:

$$i_s = AS^2 + C \frac{S^2}{b_s^{exp}} \tag{23}$$

and hence S can be calculated as:

$$S = \sqrt{\frac{i_s}{A + \dfrac{C}{b_s^{exp}}}} \tag{24}$$

Then, K_s can be obtained by using either eq. (16) or (22). In summary, the experiment has to be performed until steady-state conditions have been reached for all algorithms, but the data analysis procedure differs with the algorithm. A fitting of the infiltration model to the transient data is common to BEST-slope and BEST-intercept that differ by the use of steady-state conditions (i_s for the former algorithm and $b_{+\infty}^{end}$ for the latter one). Both of these last terms are required by BEST-steady that does not need data fitting for the transient stage of the run but relies solely on steady state.

3. BASIS OF WORKBOOK

The user-friendly analysis of BEST runs makes use of Microsoft Office EXCEL 2007 and the Microsoft Windows operating system (e.g. Windows 7). Microsoft Excel has been widely used by scientists for data collection, calculation, and analysis. Custom designed worksheet templates can easily be built, sophisticated and highly customizable macros can also be compiled using Excel Visual Basic for Applications (VBA). The workbook makes use of the Microsoft Excel Solver add-in routine. A VBA macro was written to automate creation and manipulation of Microsoft Excel Solver add-in. Before using this function, it is necessary to establish a reference to the Solver add-in. In the Visual Basic Editor, with a module active, click References on the Tools menu, and then select the Solver.xlam check box under Available References. If Solver.xlam does not appear under Available References, click Browse and open Solver.xlam in the office12\library\Solver subfolder.

4. WORKBOOK DESCRIPTION

The workbook consists of 4 worksheets: "*input*", "*back end*", "*output*" and "*charts*". In the worksheet "*input*", data for computation can be entered from column 3 and 4 (C and D) to follow. Several BEST runs can be added.

In cells from D2 to D6 (D2:D6) the user can enter the BEST run's ID, the diameter of the circular surface (cm), the number of the data describing steady-state conditions on the *I* vs. *t* plot, the initial soil water content ($m^3 m^{-3}$) and bulk density (g cm^{-3}); in cells C8:C27 and D8:D27, respectively the diameter (mm) and frequency of the soil particle size distribution (PSD), with a maximum of 20 data points, are given; in cells C29:C128 and D29:D128, respectively the time (s) and the volume (mm) of the cumulative infiltration experiment, with a maximum of 100 data points, is reported. The workbook only accepts a rigid input structure. The others worksheets are important for computation routines but they don't require an user customization.

5. COMPUTATION ROUTINES

Once the data have been entered into the Excel workbook, the first task is to perform the macro. In the worksheet ''*Input*'' the user finds the ''*EXECUTE*'' button. After a click a pop-up dialog box appears. The next step is to enter into the input dialog box the number of BEST runs to evaluate (Fig. 1). Then, it is possible to select between the different BEST algorithms by three check-boxes (by default all the options are selected). Finally, the user can chose the method for the treatment of PSD data by selecting the opportune option button (whole PSD or the method of Minasny and Mc Bractney [2006] using the USDA fractions) and click to *Execute* to run the macro.
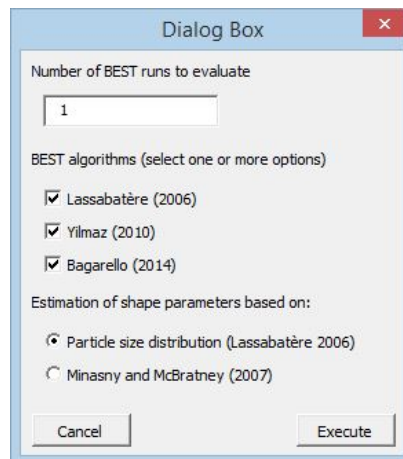

Fig. 1. Pop-up dialog box.

For a given run, the selected algorithms are applied to determine soil sorptivity, *S*. The SolverAdd function is used to minimize eq. (17). The function is repeated for a minimum of five points to a maximum of k_{tot}, i.e. the total number of collected (*t*, *I*) data points. Then, the saturated soil hydraulic conductivity, K_s, is determined. The relative error, E_r (%), is calculated to evaluate the quality of the data fitting on the transient cumulative infiltration model by the following relationship (Lassabatère et al., 2006):

$$E_r = 100 \times \sqrt{\frac{\sum_{i=1}^{k_{max}} \left[I^{exp} - I_{est} \right]^2}{\sum_{i=1}^{k_{max}} \left[I^{exp} \right]^2}} \tag{25}$$

With a For...Next structure (Visual Basic) the statements are repeated a specified number of times equal to the number of BEST runs to evaluate. At the end of the calculations, the macro directly displays the resulting parameters ordered by rows from cell A5 to X5 (A5:X5) by opening the worksheet ''*output*''.

6. WORKING EXAMPLES

A BEST run was carried out according to the methodology by Lassabatère et al. (2006). In particular, a ring of a given radius, r = 15 cm, was inserted to a short depth, d = 1 cm, into the soil surface. A known volume of water (70.7 mL) was poured in the cylinder at the start of the measurement and the elapsed infiltration time was measured. When the amount of water had completely infiltrated, an identical amount of water was poured into the cylinder and the time needed for the water to infiltrate was logged. The procedure was repeated until the difference in infiltration time between consecutive trials became negligible. The procedure is repeated for a series of 18 known volumes. An experimental cumulative infiltration, I (mm), vs. time, t (s), relationship, including a total of k_{tot} discrete points, was then deduced. The experimentally measured cumulative infiltration curve is examined to visually establish when the slope of the curve became constant (i.e. linearity in I vs. t).

Before conducting the experiment, a disturbed soil sample was collected to determine the PSD. Close to the infiltrometer ring an undisturbed soil core was collected to estimate the initial water content, θ_0 ($m^3 m^{-3}$), and the dry soil bulk density, ρ_b (g cm^{-3}). According to other investigations, the saturated water contents, θ_s ($m^3 m^{-3}$), was assumed to coincide with the estimated porosity, f ($m^3 m^{-3}$), from ρ_b (Mubarak et al., 2009, 2010; Xu et al., 2009; Yilmaz et al., 2010; Bagarello et al., 2011).

Table 1 lists the input of the BEST run analysed with the three BEST algorithms and corresponding cells references. Both procedures to estimate the shape parameters were considered, i.e. whole PSD and the method of Minasny and Mc Bractney (2006), for the runs named, respectively, "*example*" and "*example_MM*". Table 2 shows the output parameters.

Table 1. *List of input data*

row	column C	column D	column C	column D	row	column C	column D	column C	column D
BEST run's ID					Cumulative infiltration curve (t[s], I[mm])				
2	example		example_MM		29	60	4	60	4
Diameter of the circular surface (cm)					30	213	8	213	8
3	15		15		31	370	12	370	12
Number of data points describing steady-state					32	585	16	585	16
4	3		3		33	780	20	780	20
Initial water content ($m^3 m^{-3}$)					34	980	24	980	24
5	0.169		0.169		35	1164	28	1164	28
Dry soil bulk density (g cm^{-3})					36	1380	32	1380	32
6	1.2		1.2		37	1620	36	1620	36
PSD (D[mm], F)					38	1885	40	1885	40
8	2.000	1.000	2.000	1.000	39	2118	44	2118	44
9	1.000	0.962	0.050	0.500	40	2360	48	2360	48
10	0.500	0.812	0.002	0.310	41	2645	51	2645	51
11	0.250	0.649			42	2936	55	2936	55
12	0.106	0.551			43	3234	59	3234	59
13	0.053	0.514			44	3530	63	3530	63
14	0.047	0.492			45	3832	67	3832	67
15	0.033	0.481			46	4134	71	4134	71
16	0.023	0.457							
17	0.016	0.434							
18	0.012	0.422							
19	0.008	0.399							
20	0.006	0.387							
21	0.004	0.363							
22	0.003	0.340							
23	0.002	0.317							
24	0.001	0.293							

Table 2. *Output parameters*

ID	example_MM	example
k_{tot}	18	18
$\rho_b\,(m^3 m^{-3})$	1.2	1.2
$\theta_0\,(m^3 m^{-3})$	0.169	0.169
$\theta_s\,(m^3 m^{-3})$	0.547	0.547
m	0.067	0.042
n	2.144	2.088
η	16.9	25.8
steady state	3	3
slope (mm s^{-1})	0.013	0.013
intercept (mm)	17.1	17.1
Lassabatère et al. 2006		
S (mm s$^{-0.5}$)	0.495	0.495
K_s (mm s^{-1})	0.007	0.007
h_g (mm)	-39.5	-36.6
k_{step}	18	18
E_r %	1.9	1.9
Yilmaz et al. 2010		
S (mm s$^{-0.5}$)	0.477	0.477
K_s (mm s^{-1})	0.009	0.009
h_g (mm)	-28.5	-26.4
k_{step}	13	13
E_r %	2.6	2.6
Bagarello et al. 2013		
S (mm s$^{-0.5}$)	0.453	0.453
K_s (mm s^{-1})	0.008	0.008
h_g (mm)	-28.5	-26.4

7. CONCLUSIONS

In summary, the developed workbook provides a practically useful contribution to an expeditive, intensive soil hydraulic characterization, also in terms of analysis of the collected data. It was developed using the VBA language and runs under Microsoft Excel 2007. Data input and processing can be performed directly within Microsoft Excel.

The workbook is available from server at: https://bestsoilhydro.wordpress.com/downloads/.

In any case, it has to be tested extensively and unexpected behaviour of the workbook could be reported for improving the workbook.

ACKNOWLEDGMENTS

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