Multimodeling with Pedotransfer Functions.

Documentation and User Manual for PTF Calculator

(CalcPTF)

Version 3.0

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November, 2010

Abstract

Simulations of soil water flow are often carried out with parameters estimated using pedotransfer functions (PTFs), which are empirical relationships between the soil hydraulic properties and more easily obtainable basic soil properties available, for example, from soil surveys. The use of pedotransfer functions is necessary when the simulations have to be done for large-scale projects, or for pilot studies. Results of PTF applications are always uncertain, because the accuracy of pedotransfer functions outside of its development dataset is unknown. The use of several PTFs (multimodel ensemble prediction techniques) has been shown to be an efficient approach for estimating hydraulic properties within an uncertainty context. The computer program PTF calculator (CalcPTF) has been developed to estimate parameters of the Brooks and Corey and van Genuchten water retention equation to support the multimodeling approach. Seven PTFs estimate the Brooks and Corey parameters, four PTFs estimate the van Genuchten parameters, and five models fit the van Genuchten equation to pairs (capillary pressure, water content) estimated with PTFs. The PTF calculator also estimates the net capillary drive parameter of the three-parameter Parlange infiltration equation. The code is written in FORTRAN and is invoked from an Excel worksheet. Examples of input and output files are given.

Disclaimer

Contents

List of symbols

α	parameter of the van Genuchten equation corresponding approximately to the inverse of the air-entry value, (cm^{-1});
θ	the volumetric soil water content ($cm^3\ cm^{-3}$);
θ_i	the initial soil water content, ($cm^3\ cm^{-3}$);
θ_s	the saturated soil water content, ($cm^3\ cm^{-3}$);
θ_r	the residual soil water content, ($cm^3\ cm^{-3}$);
θ_{330}	the soil water content at capillary pressure of 330 cm, ($cm^3\ cm^{-3}$);
θ_{15000}	the soil water content at capillary pressure of 15000 cm, ($cm^3\ cm^{-3}$);
λ	the pore size distribution index, (dimensionless);
ρ_b	the soil bulk density, ($g\ cm^{-3}$);
σ_g	the geometric standard deviation, (cm);
ϕ	the soil porosity, ($cm^3\ cm^{-3}$);
a,b,c,d,e	empirical parameters;
$clay$	the clay content in soil, (%);
d_s	the geometric mean diameter, (cm);
f_c	the infiltrability, ($cm\ day^{-1}$);
G	the net capillary drive, (cm);
h	the capillary pressure, (cm);
h_b	the air-entry pressure, (cm);
h_w	the surface water depth, (cm);
I	the infiltrated depth, (cm);
K_s	the effective saturated hydraulic conductivity, ($cm\ day^{-1}$);
m, n	the empirical shape-defining parameters in the van Genuchten equation, (dimensionless);
OC	the organic carbon content, (%);
OM	the organic matter content, (%);
$sand$	the sand content in soil, (%);
$silt$	the silt content in soil, (%);
w	the gravimetric soil water content, ($g\ g^{-1}$).

1. **SOIL WATER RETENTION MODELS**

Soil water retention parameters are required in many applications predicting water, chemical and microbial transport in the vadose zone. In spite of major advances in the development of measurement techniques, direct determination of water retention is still expensive, time consuming, and, especially for larger scale applications, impractical. Therefore, PTFs have been developed that relate the soil hydraulic functions to more easily measurable soil properties (Pachepsky and Rawls, 2004; Vereecken et al., 2010). Two four-parameters water retention models are used commonly in the transport models: Brooks-Corey and van Genuchten equation.

The Brooks-Corey (Brooks and Corey, 1964) model establishes a power relationship between soil volumetric water content θ and capillary pressure h in form:

$$\frac{\theta-\theta_r}{\phi-\theta_r}=\begin{cases}\left(\frac{h_b}{h}\right)^{\lambda}, & h>h_b\\ 1, & h\le h_b\end{cases} \qquad [1]$$

where ϕ is the soil porosity, cm^3 cm^{-3}; θ_r is the residual water content, cm^3 cm^{-3}; h_b is air-entry pressure, cm; and λ is pore size distribution index.

The van Genuchten water retention equation (van Genuchten, 1980) is:

$$\frac{\theta-\theta_r}{\theta_s-\theta_r}=\frac{1}{\left[1+(\alpha h)^n\right]^m} \qquad [2]$$

where θ_s is the saturated water content, cm^3 cm^{-3}; α is a parameter corresponding approximately to the inverse of the air-entry value, cm^{-1}; m and n are empirical shape-defining parameters. Parameter m in the van Genuchten model is often computed as: m=1-1/n.

There are two general methods to derive the water retention parameters. The Brook-Corey and van Genuchten parameters can be obtained by fitting equations [1] and [2] to pairs (h,θ). They also can be estimated using basic soil properties such as soil texture, bulk density, organic carbon content, etc.

2. PEDOTRANSFER FUNCTIONS TO ESTIMATE SOIL WATER RETENTION

Measurements to obtain the water retention data and to derive parameters of models [1] or [2] are notoriously resource-demanding. Therefore, simulations of soil water flow are often carried out with parameters estimated using pedotransfer functions (PTFs), which are empirical relationships between the soil hydraulic properties and more easily obtainable basic soil properties available, for example, from soil surveys. The use of pedotransfer functions is necessary when the simulations have to be done for large-scale projects, or for pilot studies (Pachepsky and Rawls, 2004). Applying pedotransfer functions always introduces substantial uncertainty, since the accuracy of pedotransfer functions outside of its development dataset is unknown. The use of several PTFs (multi-model ensemble prediction techniques) has been shown to be an efficient approach for estimating hydraulic properties within an uncertainty context (Guber et al., 2006). The multimodeling approach combines predictions with the different PTFs to either derive a single set of hydraulic parameters or aggregate the output of model runs that were obtained for each of the individual PTFs. For example, (Guber et al., 2009) used 19 published PTFs and the HYDRUS-1D code to simulate the field soil water regime, and combined the simulation results of the 19 different individual models to obtain the best accuracy in terms of soil moisture content at several depths.

The computer program PTF calculator (CalcPTF) has been developed to estimate parameters of the Brooks and Corey (1964) and van Genuchten (1980) water retention equation in support of the multimodeling approach. Sixteen PTFs developed worldwide from large databases were included (Table 1). Seven PTFs (PTF1 - PTF7) estimate parameters of the Brooks-Corey equation [1], four PTFs (PTF8 - PTF11) estimate parameters of the van Genuchten equation [2], and nine PTFs estimate water content at selected capillary pressures. For five of nine PTFs (PTF12 – PTF16) which compute more than 2 pairs of (h,θ) we fit Eq. [2] to the estimated water contents at selected capillary pressures to derive the van Genuchten parameters. The other four PTFs (PTF17 – PTF20) compute θ values for capillary pressures of 330 and 15000 cm.

In the equations below, the symbols w and θ denote gravimetric (g g^{-1}) and volumetric (cm^{3}cm^{-3}) water contents, respectively, the subscripts 330 and 15000 indicate the capillary pressures in cm, *clay* and *sand* denote percentages of textural fractions according the USDA textural classification, OM is the organic matter content (%), OC is the organic carbon content (%), ρ_b is the bulk density (g cm^{-3}), other symbols are defined as they appear. The PTFs are listed in the order of increasing number of soil properties used as their input.

2.1. Equations to estimate the Brooks-Corey parameters

Saxton et al. (1986) developed the following equations to estimate the Brooks-Corey parameters (Eq.[1]) from sand and clay content. They set the value of the residual water content in Eq. [2] equal to zero and transformed the original equation to:

$$h = A\theta^{B} \qquad [3]$$

where

$$A=100\cdot\exp(-4.396-0.0715\cdot clay-0.000488\cdot sand^2-0.00004285\cdot sand^2\cdot clay) \qquad [4]$$

$$B=-3.140-0.00222\cdot clay^2-0.00003484\cdot sand^2\cdot clay \qquad [5]$$

Campbell and Shiozava (1992) used sand, clay content and soil bulk density to compute the Brooks-Corey parameters. The value of the residual water content in Eq. [1] was set equal to zero to transform the Brooks-Corey model to:

$$h = h_b\left(\theta/\theta_s\right)^{-b} \qquad [6]$$

The parameters in ([6]), estimated from two data sets for British soils, were found to be

$$\begin{aligned} h_{es} &= -0.05 d_g^{-1/2} \\ b &= -20 h_{es} + 0.2\sigma_g \end{aligned} \qquad [7]$$

where the value of h_{es} corresponds to the air entry pressure at a standard bulk density, ρ_b of 1.3 g cm^{-3}. The proposed adjustment for bulk density is

$$h_b = h_{es}\left(\rho_b/1.3\right)^{0.67b} \qquad [8]$$

The geometric mean diameter d_s and geometric standard deviation are given by

$$d_g=\exp(-0.80 - 0.0317 silt - 0.0761 clay) \qquad [9]$$

$$\sigma_g=\exp(0.133 silt +0.477 clay - \ln^2 d_g)^{1/2}$$

Table 1. List of PTFs with input soil properties

#	PTF	Region	Number of samples	Model	Sand	Silt	Clay	OC	BD	Depth
					%	%	%	%	g cm^{-3}	cm
1	Saxton et al., 1986	USA, nationwide	5320	BC	+		+		+	
2	Campbell and Shiosawa, 1992	No particular	6 soils	BC	+		+		+	
3	Rawls and Brakensiek, 1985	USA, nationwide	5320	BC	+		+		+	
4	Williams et al., 1992	Australia	196	BC	+		+		+	
5	Williams et al., 1992	Australia	196	BC	+		+	+	+	
6	Oosterveld and Chang, 1980	Canada, Alberta	298	BC	+		+		+	+
7	Mayr and Jarvice, 1999	UK	306	BC	+	+	+	+	+	
8	Wösten et al., 1999	Europe	4030	VG	+	+	+			+
9	Varallyay et al., 1982	Hungary	230	VG			+		+	
10	Vereecken et al., 1989	Belgium	182	VG	+		+	+	+	
11	Wösten et al., 1999	Europe	4030	VG		+	+	+	+	+
12	Tomasella and Hodnett, 1998	Brazil	196	WH -> VG		+	+	+		
13	Rawls et al., 1982*	USA, nationwide	5320	WH -> VG	+	+	+	+	+	
14	Gupta and Larson, 1979	Central USA	43 sediment and soil samples	WH -> VG	+	+	+	+	+	
15	Rajkai and Varallyay, 1992	Hungary	270	WH -> VG	+		+	+	+	
16	Rawls et al., 1983*	USA, nationwide	5320	WH -> VG	+	+	+	+	+	
17	Peterson et al., 1968	Pennsylvania, USA	1267	WH			+			
18	Bruand et al., 1994	Central France	20 Bt horizons	WH			+			
19	Canarache, 1993	Romania	Unknown	WH			+		+	
20	Hall et al., 1977	UK, England, Wales	261	WH	+	+	+		+	

BC is the Brooks and Corey model (Eq.[1])

VG is the van Genuchten model (Eq.[2])

WH is water content at selected capillary pressures

* corrected for OM according to Nemes et al. (2009).

Rawls and Brakensiek (1985) developed the following equations to estimate the Brooks-Corey parameters in Eq. [1]:

$$h_b=\exp[5.340+0.185\cdot clay-2.484\cdot\phi-0.002\cdot clay^2-0.044\cdot sand\cdot\phi+0.001\cdot sand^2\cdot\phi^2-0.009\cdot clay^2\cdot\phi^2-\\ 0.00001\cdot sand^2\cdot clay+0.009\cdot clay^2\cdot sand-0.0007\cdot sand^2\cdot\phi\\ 0.000005\cdot clay^2\cdot sand-0.500\cdot\phi^2\cdot clay] \qquad [10]$$

$$\lambda=\exp[-0.784+0.018\cdot sand-1.062\cdot\phi-0.00005\cdot sand^2-0.003\cdot clay^2+1.111\cdot\phi^2-0.031\cdot sand\cdot\phi\\ +0.0003\cdot sand^2\cdot\phi^2-0.006\cdot clay^2\cdot\phi^2-0.000002\cdot sand^2\cdot clay+0.008\cdot clay^2\cdot\phi\\ -0.007\cdot\phi^2\cdot \mathrm{clay}] \qquad [11]$$

$$\theta_r=-0.018+0.0009\cdot sand+0.005\cdot clay+0.029\cdot\phi-0.0002\cdot clay^2-0.001\cdot sand\cdot\phi-\\ 0.0002\cdot clay^2\cdot\phi^2+0.0003\cdot clay^2\cdot\phi-0.002\cdot\phi^2\cdot clay \qquad [12]$$

Williams et al. (1992) transformed Eq. [1] with $\theta_\mathrm{r}=0$ to the logarithmic form:

$$\ln\theta=A+B\ln h \qquad [13]$$

and applied it to an Australian database.

Different pedotransfer equations were developed in their work for different types of available data of basic properties. The equations

$$\mathrm{A}=1.839+0.257\cdot\ln(clay)+0.381\cdot 2.0-0.0001\cdot sand^2 \qquad [14]$$

$$\mathrm{B}=-0.303+0.093\cdot\ln(\rho_b)+0.0565\cdot\ln(clay)-0.00003\cdot sand^2 \qquad [15]$$

were suggested when no information about the organic matter content was available, and the equations:

$$A=2.57+0.238\cdot\ln(clay)-0.000192\cdot sand^2-0.0137\cdot sand-0.0926\cdot\ln(\mathrm{OM})+0.0412\cdot\mathrm{OM} \qquad [16]$$

$$B=-0.403+0.0871\cdot\ln(clay)-0.00077\cdot sand \qquad [17]$$

for cases when data on the organic matter are available.

Oosterveld and Chang (1980) used a Canadian database and transformed Eq. [1] with $\theta_\mathrm{r}=0$ to the form:

$$\theta=0.01\cdot\rho_b\cdot(35.367+0.644\cdot clay-0.251\cdot sand-0.045\cdot\mathrm{D})\cdot h^{-0.190} \qquad [18]$$

where D is the mean depth of the sample in centimeters.

Mayr and Jarvis (1999) set θ_r=0 and porosity ϕ equal to the saturated water θ_s in the Brooks-Corey equation, and combined this equation for the dry range of soil water retention curve

$$\theta = \theta_s (h/a)^{-1/b} \qquad \theta < \theta_i \qquad [19]$$

with a parabolic equation for the wet range:

$$\theta = \theta_s - \frac{\theta_s h^2 (1-\theta_i/\theta_s)}{a^2 (\theta_i/\theta_s)^{-2b}} \qquad \theta \geq \theta_i \qquad [20]$$

The water content θ_i and the equivalent capillary pressure h_i at the matching point are given by:

$$\theta_i = \frac{2b\theta_s}{1+2b} \qquad [21]$$

and

$$h_i = a\left(\frac{2b}{1+2b}\right)^{-b} \qquad [22]$$

Pedotransfer functions developed by Mayr and Jarvis (1999) from a Scandinavian dataset were:

$$\log(a)=-4.9840297533+0.0509226283\cdot \mathit{sand}+0.1575152771\cdot \mathit{silt}+0.1240901644\cdot \rho_b -0.1640033143\cdot \mathrm{OC}-0.0021767278\cdot \mathit{silt}^2+0.0000143822\cdot \mathit{silt}^3+0.0008040715\cdot \mathit{clay}^2 +0.0044067117\cdot \mathrm{OC}^2) \qquad [23]$$

$$\log(1/b)=-0.8466880654-0.0046806123\cdot \mathit{sand}+0.0092463819\cdot \mathit{silt}-0.4542769707\cdot \rho_b -0.0497915563\cdot \mathrm{OC}+0.0003294687\cdot \mathit{sand}^2 +0.000001689056\cdot \mathit{sand}^3+0.0011225373\cdot \mathrm{OC}^2 \qquad [24]$$

$$\theta_s = 0.2345971971+0.0046614221\cdot \mathit{sand}+0.0088163314\cdot \mathit{silt}+0.0064338641\cdot \mathit{clay}- 0.3028160229\cdot \rho_b +0.179762\cdot 10^{-4}\cdot \mathit{sand}^2-0.3134631\cdot 10^{-4}\cdot \mathit{silt}^2 \qquad [25]$$

2.2. Equations to estimate the van Genuchten parameters

Wösten et al. (1999) analyzed the all-Europe database HYPRES and derived the class pedotransfer functions. These PTFs represent the van Genuchten parameters obtained by fitting the equation [2] to geometric mean water contents for each of 5 textural groups (Table 2).

Table 2. van Genuchten parameters for the fits on the geometric mean curves

Soil texture	Definition	θ_r	θ_s	α	n	m
		Topsoils				
Coarse	*clay*<18% and *sand*>65%	0.025	0.403	0.0383	1.3774	0.2740
Medium	18%<*clay*<35% and 15%<*sand* or *clay*<18% and 15%<*sand*<65%	0.010	0.439	0.0314	1.1804	0.1528
Medium fine	*clay*<35% and *sand*<15%	0.010	0.430	0.0083	1.2539	0.2025
Fine	35%<*clay*<60%	0.010	0.520	0.0367	1.1012	0.0919
Very Fine	60%<*clay*	0.010	0.614	0.0265	1.1033	0.0936
		Subsoils				
Coarse	*clay*<18% and *sand*>65%	0.025	0.366	0.0430	1.5206	0.3424
Medium	18%<*clay*<35% and 15%<*sand* or *clay*<18% and 15%<*sand*<65%	0.010	0.392	0.0249	1.1689	0.1445
Medium fine	*clay*<35% and *sand*<15%	0.010	0.412	0.0082	1.2179	0.1789
Fine	35%<*clay*<60%	0.010	0.481	0.0198	1.0861	0.0793
Very Fine	60%<*clay*	0.010	0.538	0.0168	1.0730	0.0680

Same authors (Wösten et al. 1999) derived the regression equations to estimate the van Genuchten parameters from soil texture, organic carbon content and soil bulk density:

$$\begin{aligned}\theta_s = {} & 0.7919 + 0.001691\cdot clay - 0.29619\cdot\rho_b - 0.000001491\cdot silt^2 + 0.0000821\cdot \mathrm{OM}^2 + 0.02427/clay \\ & + 0.01113/silt + 0.01472\cdot\ln(silt) - 0.0000733\cdot\mathrm{OM}\cdot clay - \\ & 0.000619\cdot\rho_b\cdot clay - 0.001183\cdot\rho_b\cdot\mathrm{OM} - 0.0001664\cdot topsoil\cdot silt \qquad [27]\end{aligned}$$

$$\begin{aligned}\alpha = {} & \exp[-14.96 + 0.03135\cdot clay + 0.0351\cdot silt + 0.646\cdot\mathrm{OM} + 15.29\cdot\rho_b - 0.192\cdot topsoil \\ & - 4.671\cdot\rho_b^2 - 0.000781\cdot clay^2 - 0.00687\cdot\mathrm{OM}^2 + 0.0449/\mathrm{OM} + 0.0663\cdot\ln(silt) + \\ & 0.1482\cdot\ln(\mathrm{OM}) - 0.04546\cdot\rho_b\cdot silt - 0.4852\cdot\rho_b\cdot\mathrm{OM} + 0.00673\cdot topsoil\cdot clay] \qquad [28]\end{aligned}$$

$$\begin{aligned}n = {} & 1.+\exp[-25.23 - 0.02195\cdot clay + 0.0074\cdot silt - 0.1940\cdot\mathrm{OM} + 45.5\cdot\rho_b - 7.24\cdot\rho_b^2 + \\ & 0.0003658\cdot clay^2 + 0.002885\cdot\mathrm{OM}^2 - 12.81/\cdot\rho_b - 0.1524/silt - 0.01958/\mathrm{OM} - \\ & 0.2876\cdot\ln(silt) - 0.0709\cdot\ln(\mathrm{OM}) - 44.6\cdot\ln(\rho_b) - 0.02264\cdot\rho_b\cdot clay + 0.0896\cdot\rho_b\cdot\mathrm{OM} \\ & + 0.00718\cdot topsoil\cdot clay \qquad [29]\end{aligned}$$

where topsoil is an ordinal variable having the value of 1 or of 0. Parameter m in Eq. [2] was computed as $1-1/n$.

Varallyay et al. (1982) applied the van Genuchten equation with $m=1$ and $\theta_r = 0$ to the Hungarian national database and found the following regression equations for A-horizons:

$$\theta_s = 0.01(-56.4\cdot\rho_b + 0.00205\cdot clay^2 + 123.79) \qquad [30]$$

$$n = 0.336\cdot\rho_b - 0.053 \qquad [31]$$

$$\alpha = 10^{\,0.417-0.0427\cdot\rho_b\cdot\mathrm{clay}\,-\,1.51\cdot\rho_b} \qquad [32]$$

Vereecken et al. (1989) used a Belgian dataset to develop the following pedotransfer functions for the van Genuchten equation with m=1:

$$\theta_s = 0.81 - 0.283\cdot\rho_b + 0.001\cdot clay \qquad [33]$$

$$\theta_r = 0.015 + 0.005\cdot clay + 0.014\cdot \mathrm{OC} \qquad [34]$$

$$\alpha = \exp(-2.486 + 0.025\cdot sand - 0.351\cdot clay - 2.617\cdot\rho_b - 0.023\cdot clay\,) \qquad [35]$$

$$n = \exp(0.053 - 0.009\cdot sand - 0.013\cdot clay + 0.00015\cdot sand^2) \qquad [36]$$

2.3. Equations to estimate the soil water content at selected capillary pressures

The following five PTFs were developed to estimate water contents at several selected capillary pressures that allowed fitting the van Genuchten equation [2] to pairs (h,θ). The fitting code (VGpar.for) is based on the optimization procedure from the CFITM program (van Genuchten, 1980) developed to determine transport parameters from solute displacement experiments.

Tomasella and Hodnett (1998) studied Brazilian soils and derived regression parameters for water contents θ at nine capillary pressures h:

$$\theta = 0.01\cdot(a\cdot \mathrm{OC} + b\cdot silt + c\cdot clay + d) \qquad [37]$$

Table 3. Coefficients of multiple linear regressions in Eq.[37]

h, cm	*a*	*b*	*c*	*d*
0	2.24	0.298	0.159	37.937
10	0	0.53	0.255	23.839
30	0	0.552	0.262	18.495
60	0	0.576	0.3	12.333
100	0	0.543	0.321	9.806
330	0	0.426	0.404	4.046
1000	0	0.369	0.351	3.198
5000	0	0.258	0.361	1.567
15000	0	0.15	0.396	0.91

Rawls et al. (1982) used the US Cooperative Soil Survey Database to develop 12 regression equations to relate the soil water contents at 12 capillary pressures to sand, clay and organic matter contents (Table 4). A similar set of equations was later developed to use knowledge of the bulk density along with the sand, clay and organic matter contents (Rawls et al., 1983; Table 5).

Table 4. Coefficients of the linear regression equation to predict volumetric soil water content at specific capillary pressure: $\theta = a + b \cdot sand + c \cdot silt + d \cdot clay + e \cdot \mathrm{OC}$ (after Rawls et al., 1982)

h, cm	*a*	*b*	*c*	*d*	*e*
100	0.4118	-0.0030	0	0.0023	0.0317
200	0.3121	-0.0024	0	0.0032	0.0314
330	0.2576	-0.0020	0	0.0036	0.0299
600	0.2065	-0.0016	0	0.0040	0.0275
1000	0.0349	0	0.0014	0.0055	0.0251
2000	0.0281	0	0.0011	0.0054	0.0200
4000	0.0238	0	0.0008	0.0052	0.0190
7000	0.0216	0	0.0006	0.0050	0.0167
10000	0.0205	0	0.0005	0.0049	0.0154
15000	0.0260	0	0	0.0050	0.0158

Table 5. Coefficients of the linear regression equation to predict volumetric soil water content at specific capillary pressure: $\theta = a + b \cdot sand + c \cdot clay + d \cdot \mathrm{OC} + e \cdot \rho_b$ (after Rawls et al., 1983)

h, cm	*a*	*b*	*c*	*d*	*e*
200	0.4180	-0.0021	0.0035	0.0232	-0.0859
330	0.3486	-0.0018	0.0039	0.0228	-0.0738
600	0.2819	-0.0014	0.0042	0.0216	-0.0612
1000	0.2352	-0.0012	0.0043	0.0202	-0.0517
2000	0.1837	-0.0009	0.0044	0.0181	-0.0407
4000	0.1426	-0.0007	0.0045	0.0160	-0.0315
7000	0.1155	-0.0005	0.0045	0.0143	-0.0253
10000	0.1005	-0.0004	0.0045	0.0133	-0.0218
15000	0.0854	-0.0004	0.0044	0.0122	-0.0182

Gupta and Larson (1979) used a subset of the US National Cooperative Survey database to derive predictive equations for the volumetric water content at twelve capillary pressures:

$$\theta = a \cdot sand + b \cdot silt + c \cdot clay + d \cdot \mathrm{OC} + e \cdot \rho_b \qquad [38]$$

Table 6. Coefficients of the linear regression equation [40] to predict volumetric soil water content at specific capillary pressure

h, cm	*a*	*b*	*c*	*d*	*e*
40	7.053	10.242	10.07	6.333	-321.2
70	5.678	9.228	9.135	6.103	-269.6
100	5.018	8.548	8.833	4.966	-242.3
200	3.89	7.066	8.408	2.817	-187.8
330	3.075	5.886	8.039	2.208	-143.4
600	2.181	4.557	7.557	2.191	-92.76
100	1.563	3.62	7.154	2.388	-57.59
200	0.932	2.643	6.636	2.717	-22.14
400	0.483	1.943	6.128	2.925	-2.04
700	0.214	1.538	5.908	2.855	15.3
1000	0.076	1.334	5.802	2.653	21.45
15000	-0.059	1.142	5.766	2.228	26.71

Rajkai and Varallyay (1992) analyzed the Hungarian national database to obtain a nonlinear regression for ten specific capillary pressures:

$$\theta = b_0 + b_1\mathrm{X}_1 + b_2\mathrm{X}_2 + b_3\mathrm{X}_1\mathrm{X}_2 + b_4\mathrm{X}_1^2 + b_5\mathrm{X}_2^2 \qquad [39]$$

We used only eight capillary pressures in the CalcPTF (Table 7).

Table 7. Coefficients and variables in the nonlinear regression equation [41] to predict volumetric soil water content at specific capillary pressure

h, cm	X_1	X_2	b_0	b_1	b_2	b_3	b_4	b_5
0	ρ_b	*silt*	89.75	-31.39	0	0.03	0	0
3	ρ_b	*sand*	85.05	-27.17	0	-0.024	0	0
10	ρ_b	*sand*	78.58	-23.94	0	-0.025	0	0
32	ρ_b	*clay+silt*	69.78	-21.74	0	0	0	0.0011
501	*clay+silt*	*sand/silt*	20.87	0.29	-0.83	0.03	0	0.0051
2512	*clay+silt*	OM	2.19	0.52	3.93	-0.07	0	0
15849	*clay+silt*	OM	1.39	0.36	0	0	0	0.22
1258925	*clay*	OM	0.73	0	0.32	0	0.0018	0

The following four PTF estimate volumetric water content at capillary pressure of 330 cm and 15000 cm and are not used to compute parameters in Eq.[1] and Eq.[2].

Peterson et al. (1968) worked with the Pennsylvania soil database. Their equations are:

$$\theta_{330} = 0.01\cdot(11.83+0.96\cdot clay-0.008\cdot clay^2) \qquad [40]$$

$$\theta_{15000} = 0.01\cdot(1.74+0.76\cdot clay - 0.005\cdot clay^2) \qquad [41]$$

Bruand et al. (1994) for soils in central France estimated the volumetric water content at the same capillary pressures as:

$$\theta_{330} = (0.043+0.004\cdot clay)/(0.471+0.00411\cdot clay) \qquad [42]$$

$$\theta_{15000} = (0.008+0.00367\cdot clay)/(0.471+0.00411\cdot clay) \qquad [43]$$

Canarache (1993) applied regression analysis to the Romanian national database to obtain the predictive equations:

$$\theta_{330}=0.01\cdot\rho_b\cdot(2.65+1.105\cdot clay-0.01896\cdot clay^2+0.0001678\cdot clay^3 +15.12\cdot\rho_b-6.745\cdot\rho_b^2-0.1975\cdot clay\cdot\rho_b) \qquad [44]$$

$$\theta_{15000}=0.01\cdot\rho_b\cdot(0.2805\cdot clay+0.0009615\cdot clay^2) \qquad [45]$$

Hall et al. (1977) analyzed a subset of British Soil Survey data and derived the equations

$$\theta_{330}=0.01\cdot(20.81+0.45\cdot clay+0.13\cdot \mathrm{silt}-5.95\cdot\rho_b) \qquad [46]$$

$$\theta_{15000}=0.01\cdot(1.48+0.84\cdot clay-0.0055\cdot clay^2) \qquad [47]$$

3. Estimating the net capillary drive parameter in the Parlange infiltration equation

The PTFs listed in sections 2.1 and 2.2 can be also used to compute the net capillary drive parameter in the equation describing water infiltration into unsaturated soil (Parlange et al., 1982). The general one-layer model for infiltrability f_c, as a function of infiltrated depth I, is:

$$f_c = K_s\left[1+\frac{\sigma}{\exp(\sigma I/B)-1}\right] \qquad [48]$$

where B is combining the effects of net capillary drive G, surface water depth h_w, and unit storage capacity $\theta_s-\theta_i$:

$$B=(G+h_w)(\theta_s-\theta_i) \qquad [49]$$

the parameter σ represents the soil type, and θ_i is initial soil water content.

The equation [48] is used in the KINEROS2 model describing sediment (Woolhiser et al., 1990) and bacteria (Guber et al., 2010) transport with overland water flow and requires 4 basic parameters to describe the infiltration properties of a soil: the field effective saturated hydraulic conductivity K_s, the net capillary drive G, and the saturated water content θ_s. The value of σ is set equal to 0.85 in the KINEROS2 model, while the other three parameters are estimated for 11 soil textural classes (Rawls et al., 1982).

The KINEROS2 model uses class PTFs (Pachepsky and Rawls, 2004) to estimate the net capillary drive. The CalcPTF is a continuous PTF based on the Morel-Seytoux et al. (1996) equations computing the net capillary drive from the Brooks-Corey and van Genuchten parameters. For the Brooks-Corey model (Eq.[1]) the net capillary drive G is:

$$G = h_b \frac{2+3\lambda}{1+3\lambda} \qquad [50]$$

and for the van Genuchten model (Eq.[2]) G is:

$$G = \frac{0.046m + 2.07m^2 + 19.5m^3}{\alpha(1+4.7m+16m^2)} \qquad [51]$$

4. PROGRAM DESCRIPTION

4.1. File list

A FORTRAN code has been written to implement the CalcPTF. The program includes 4 files which have to be located in the C:\PTF folder:

1. *CalcPTF.xls* is a Microsoft Office Excel file containing list of PTFs with input parameters, references to the original publications, input data and results in form of Excel datasheet and graphics.
2. *PTFG.exe* is an executable file computing and saving results of PTF estimations.
3. *PTFG.for* is a FORTRAN main program handling input and output data and performing PTF computations.
4. *VGpar.for* is a subroutine fitting the van Genuchten parameters to pairs of (h,θ) estimated with four PTFs (PTF17 – PTF20).

The *PTFG.exe* file can be run from PTFG.xls file using macros *PTFG* or independently from Windows Explorer. The run from *CalcPTF.xls* is preferable, because it allows preparing input data and analyzing results of computations within a single file.

4.2. Input data

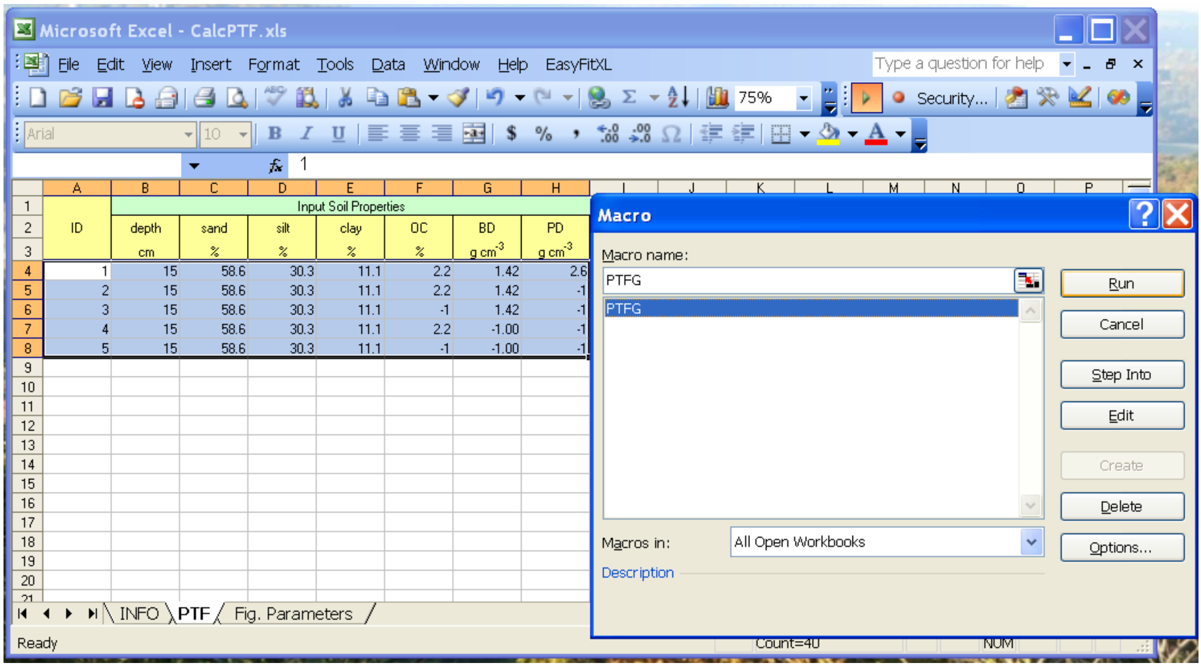
The input data for *PTFG.exe* are given in input file *ptf.in*. The input file contains soil properties used in PTFs and has to be placed into the same C:\PTF folder. The *PTFG.exe* information that needs to be supplied in *ptf.in* file is:

Sample ID, Depth (cm), Sand (%), Silt (%), Clay (%), OC (%), BD (g cm^{-3}), PD (g cm^{-3})

Input data for each sample starts from new line and can be separated using space or comma within the line. Up to 100 lines (samples) can be processed within one *PTFG.exe* run. Any soil property can be omitted if not measured. The missed values should be entered as "-1" in *ptf.in* file. The soil particle density is set to 2.65 g cm^{-3} by default, but can be changed if known and different. The *PTFG.exe* module uses only PTFs, which have all necessary input data (Table 1). Parameter values of "-1" are generated by the code for PTFs which input data are lacking.

The simplest way to prepare data and run *PTFG.exe* is to fill columns "A-H" of the worksheet "PTF", to select all or some lines in the data table using the regular Excel selection pointer ✚ and to run the *PTFG* macro. Note, that only data from selected will be saved in *ptf.in* file and used in computations.

Figure 1. Input data and Macro window to run *PTFG.exe* module



fx 1

ID	Input Soil Properties						
	depth cm	sand %	silt %	clay %	OC %	BD g cm^{-3}	PD g cm^{-3}
1	15	58.6	30.3	11.1	2.2	1.42	2.6
2	15	58.6	30.3	11.1	2.2	1.42	-1
3	15	58.6	30.3	11.1	-1	1.42	-1
4	15	58.6	30.3	11.1	2.2	-1.00	-1
5	15	58.6	30.3	11.1	-1	-1.00	-1

Macro name: PTFG

PTFG

Macros in: All Open Workbooks

4.3. Output data

1. The *PTFG.exe* module creates new output files as follows. The *Temp.dat* file is a temporary file with computed parameters of the Brooks-Corey and van Genuchten water retention models. The *PTFG* macros transfers these data from *Temp.dat* to the *PTF* worksheet in columns according to the PTFs and rows corresponding to the input data selected in this worksheet data. These results can be seen graphically in *Fig.Parameters* worksheet of *CalcPTF file*.
2. *The WR.par* file is an output file containing parameters of the Brooks-Corey and van Genuchten water retention models in the form suitable for the HYDRUS family models (www.pc-progress.com). Specifically parameter h_b in Eq.[1] is replaced with its inverse value $\alpha = 1/\ h_b$ as it used in the HYDRUS model. The PTFs and depths with no output data are skipped in the *WR.par* file.
3. *WC.out* is the output file containing water contents computed at capillary pressures of 330 and 15000 cm using PTF16 - PTF20 (Table 1).

4.4. Example

This example demonstrates CalcPTF computations for samples with different number of measured soil properties. Input data for four samples are stored in *PTF* worksheet of *CalcPTF.xls* (Figure 1.). We ran macros *PTFG* to save data into *ptf.in* data file, start *PTFG.exe* executable module and transfer results into *PTF* worksheet. The *PTFG* macros created file *ptf.in* with input data:

```
1 15 58.6 30.3 11.1 2.2 1.42 2.6
2 15 58.6 30.3 11.1 2.2 1.42 -1
3 15 58.6 30.3 11.1 -1 1.42 -1
4 15 58.6 30.3 11.1 2.2 -1 -1
5 15 58.6 30.3 11.1 -1 -1 -1
```

These data are processed by *PTFG.exe* executable module and results are saved in file *WR.par* and *WC.out*:

File *WR.par*:

Brooks and Corey (1964) water retention model

```
Saxton et al., 1986
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.45385   0.11593   0.21090
  2   15.   0.00000   0.46415   0.12895   0.21090
  3   15.   0.00000   0.46415   0.12895   0.21090
Campbell and Shiosawa, 1992
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.45385   0.04192   0.22767
  2   15.   0.00000   0.46415   0.04192   0.22767
  3   15.   0.00000   0.46415   0.04192   0.22767
Rawls and Brakensiek, 1985
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.06261   0.45385   0.07489   0.38180
  2   15.   0.06219   0.46415   0.07854   0.37871
  3   15.   0.06219   0.46415   0.07854   0.37871
Williams et al., 1992
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.45385   0.05211   0.23742
  2   15.   0.00000   0.46415   0.05728   0.23742
  3   15.   0.00000   0.46415   0.05728   0.23742
Williams et al., 1992
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.45385   0.23190   0.23848
  2   15.   0.00000   0.46415   0.25480   0.23848
Oosterveld and Chang, 1980
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.45385   0.18365   0.19000
  2   15.   0.00000   0.46415   0.20669   0.19000
  3   15.   0.00000   0.46415   0.20669   0.19000
Mayr and Jarvice, 1999
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.44926   0.32949   0.45001
  2   15.   0.00000   0.44926   0.32949   0.45001

van Genuchten (1980) water retention model
Wosten et al., 1999
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.01000   0.39200   0.02490   1.16890
  2   15.   0.01000   0.39200   0.02490   1.16890
  3   15.   0.01000   0.39200   0.02490   1.16890
  4   15.   0.01000   0.39200   0.02490   1.16890
  5   15.   0.01000   0.39200   0.02490   1.16890
Varallyay et al., 1982
 ID  Depth    ThetaR    ThetaS    alpha       n
  1   15.   0.00000   0.43865   0.00398   0.42412
  2   15.   0.00000   0.43865   0.00398   0.42412
```

```
   3   15.   0.00000   0.43865   0.00398   0.42412
Vereecken et al., 1989
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.10130   0.41924   0.00732   0.90158
   2   15.   0.10130   0.41924   0.00732   0.90158
Wosten et al., 1999
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.01000   0.42344   0.04355   1.22138
   2   15.   0.01000   0.42344   0.04355   1.22138
Tomasella and Hodnett, 1998
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.00000   0.53316   0.17054   1.20969
   2   15.   0.00000   0.53316   0.17054   1.20969
   4   15.   0.00000   0.53316   0.17054   1.20969
Rawls et al., 1982
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.06728   0.45412   0.02691   1.34012
   2   15.   0.06587   0.46437   0.03000   1.33471
Gupta and Larson, 1979
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.11899   0.45646   0.02491   1.42908
   2   15.   0.11698   0.46612   0.02810   1.41584
Rajkai and Varallyay, 1992
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.00000   0.44315   0.00842   1.18271
   2   15.   0.00000   0.44315   0.00842   1.18271
Rawls et al., 1983
 ID  Depth    ThetaR    ThetaS    alpha       n
   1   15.   0.05738   0.45387   0.04820   1.29281
   2   15.   0.05703   0.46417   0.05321   1.29156
```

File *WC.out*:

```
Peterson et al., 1968
Z/P,cm    330.0  15000.0
 15.0    0.215    0.096
 15.0    0.215    0.096
 15.0    0.215    0.096
 15.0    0.215    0.096
 15.0    0.215    0.096

Bruand et al., 1994
Z/P,cm     330.0   15000.0
 15.0     0.169     0.094
 15.0     0.169     0.094
 15.0     0.169     0.094
```

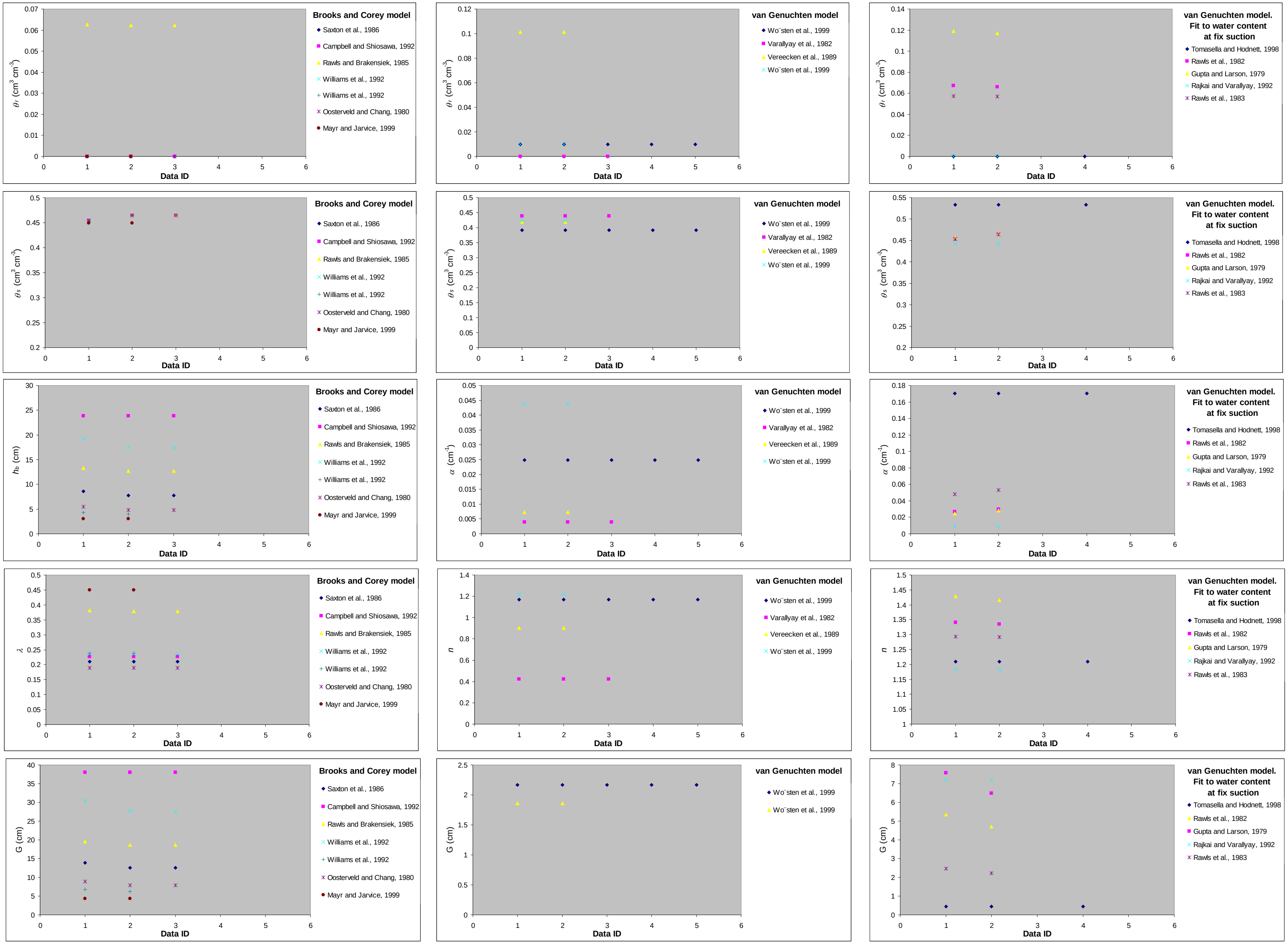
```
 15.0     0.169     0.094
 15.0     0.169     0.094

Canarache, 1993
Z/P,cm    330.0  15000.0
 15.0    0.249    0.046
 15.0    0.249    0.046
 15.0    0.249    0.046

Hall et al., 1977
Z/P,cm    330.0  15000.0
 15.0    0.213    0.101
 15.0    0.213    0.101
 15.0    0.213    0.101
```

Output parameters are also saved in the worksheet PTF and plotted in the worksheet *Fig. Parameters* of *CalcPTF.xls* file (Fig. 2). Note, that the Brooks-Corey and van Genuchten parameters are set to -1 for PTFs that have missing input soil properties.

Figure 2. Example of parameter computation for 4 soil samples using CalcPTF



REFERENCES

1. Baumer, O.M. 1992. Predicting unsaturated hydraulic parameters. p. 341–354. In M.Th. van Genuchten et al .(Ed.) Proc. Int.Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, Riverside.
2. Brooks, R.H., and A.J. Corey. 1964. Hydraulic properties of porous media. Hydrol. Paper 3. Colorado State Univ., Fort Collins.
3. Bruand, A., D. Baize, and M. Hardy. 1994. Prediction of water retention properties of clayey soils: Validity of relationships using a singlesoil characteristic. Soil Use Manage. 10:99–103.
4. Campbell, G.S., and S. Shiozawa. 1992. Prediction of hydraulic properties of soils using particle size distribution and bulk density data. p. 317–328. In M.Th. van Genuchten et al (ed.) Proc. Int.Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, Riverside
5. Canarache, A. 1993. Physical-technological maps—A possible product of soil survey for direct use in agriculture. Soil Technol. 6:3–16.
6. Guber, A.K., Ya.A. Pachepsky, M.Th. van Genuchten, W.J. Rawls, J. Simunek, D. Jacques, T.J. Nicholson, and R.E. Cady. 2006. Field-scale water flow simulations using ensembles of pedotransfer functions for soil water retention. Vadose Zone Journal, 5:234–247.
7. Guber, A.K., Ya.A. Pachepsky, M. Th. van Genuchten, J. Šimůnek, D. Jacques, A. Nemes, T.J. Nicholson, and R.E. Cady. 2009. Multimodel simulation of water flow in a field soil using pedotransfer functions. Vadose Zone J. 8:1–10.
8. Guber, A.K., Y.A. Pachepsky, A.M. Yakirevich , D.R. Shelton, A.M. Sadeghi, D.C. Goodrich, C.L. Unkrich. 2010. Uncertainty in modeling of Faecal Coliform overland transport associated with manure application in Maryland. Hydrological Processes (in review).
9. Gupta, S.C., and W.E. Larson. 1979. Estimating soil water retention characteristics from particle-size distribution, organic matter percent, and bulk density. Water Resour. Res. 15:1633–1635.
10. Hall, D.G.M., M.J. Reeve, A.I. Thomasson, and V.F. Wright. 1977. Water retention, porosity and density of field soils. Soil Surv. Tech. Monogr. 9. Rothamsted Experimental Station, Lawes Agricultural Trust, Harpenden, UK.

11. Mayr, T., and N.J. Jarvis. 1999. Pedotransfer functions to estimate soil water retention parameters for a modified Brooks-Corey type model. Geoderma 91:1–9.
12. Morel-Seytoux, H. J., P. D. Meyer, M. Nachabe, J. Touma, M. T. van Genuchten, and R. J. Lenhard. , 1996. Parameter equivalence for Brooks-Corey and van Genuchten soil Characteristics: Preserving the effective capillary drive, Water Resour. Res., 32(5), 1251–1258.
13. Nemes, A., Timlin, D.J, Pachepsky, Ya.A.,Rawls, W.J. 2009. Evaluation of the Rawls et al. (1982) Pedotransfer Functions for their Applicability at the U.S. National Scale. SSSAJ, 73: 1638-1645.
14. Oosterveld, M., and C. Chang. 1980. Empirical relations between laboratory determinations of soil texture and moisture characteristic. Can. Agric. Eng. 22:149–151.
15. Pachepsky, Y. A., and W. J. Rawls (Eds). 2004. Development of Pedotransfer Functions in Soil Hydrology. Deelopments in Soil Scince 30. Elsevier, Amsterdam.
16. Parlange, J.-Y., I. Lisle, R.D. Braddock, and R.E. Smith. 1982. The three-parameter infiltration equation, Soil Science 133(6):337-341.
17. Petersen, G.W., R.L. Cunningham, and R.P. Matelski. 1968. Moisture characteristics of Pennsylvania soils: I. Moisture retention as related to texture. Soil Sci. Soc. Am. Proc. 32:271–275.
18. Rajkai, K., and G. Varallyay. 1992. Estimating soil water retention from simpler properties by regression techniques. p. 417–426. In M.Th. van Genuchten et al. (ed.) Proc. Int. Workshop on Indirect Methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, Riverside.
19. Rawls, W.J., and D.L. Brakensiek. 1985. Prediction of soil water properties for hydrologic modeling. p. 293–299. In E.B. Jones and T.J.Ward (ed.) Proc. Symp.Watershed Management in the Eighties, Denver, CO. 30 Apr.–1 May 1985. Am. Soc. Civil Eng., New York.
20. Rawls, W.J., D.L. Brakensiek, and B. Soni. 1983. Agricultural management effects on soil water processes. Part I. Soil water retention and Green-Ampt parameters. Trans. ASAE 26:1747–1752.
21. Rawls, W.J., D.L. Brakensiek, and K.E. Saxton. 1982. Estimation of soil water properties. Trans. ASAE 25:1316–1320.

22. Saxton, K.E., W.J. Rawls, J.S. Romberger, and R.I. Papendick. 1986. Estimating generalized soil-water characteristics from texture. Soil Sci. Soc. Am. J. 50:1031–1036.
23. Tomasella, J., and M.G. Hodnett. 1998. Estimating soil water retention characteristics from limited data in Brazilian Amazonia. Soil Sci. 163:190–202.
24. van Genuchten, M.Th. 1980.Aclosed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44:892–898.
25. van Genuchten, M.Th. 1980.Determining transport parameters from solute displacement experiments. Research report No.118, U.S. Salinity Laboratory, USDA-ARS-AR, Riverside, California.
26. Varallyay, G., Rajkai K., Ya.A. Pachepsky, and R.A. Shcherbakov. 1982. Mathematical description of soil water retention curve. (In Russian.) Pochvovedenie 4:77–89.
27. Vereecken, H., J. Maes, J. Feyen, and P. Darius. 1989. Estimating the soil moisture retention characteristics from texture, bulk density and carbon content. Soil Sci. 148:389–403.
28. Vereecken, H., M. Weynants, M. Javaux, Y. Pachepsky, M. G. Schaap, M.Th. van Genuchten. 2010. Using pedotransfer functions to estimate the van Genuchten–Mmualem soil hydraulic properties: a review. Vadose Zone J. 9:1–26.
29. Williams, J., P. Ross, and K. Bristow. 1992. Prediction of the Campbell water retention function from texture, structure, and organic matter.p. 427–442. In M.Th. van Genuchten et al (ed.) Proc. Int.Workshop on Indirect methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, Riverside.
30. Williams, J., P. Ross, and K. Bristow. 1992. Prediction of the Campbell water retention function from texture, structure, and organic matter.p. 427–442. In M.Th. van Genuchten et al (ed.) Proc. Int.Workshop on Indirect methods for Estimating the Hydraulic Properties of Unsaturated Soils. University of California, Riverside.
31. Woolhiser, D.A., R.E. Smith, and D.C. Goodrich. 1990. KINEROS, A kinematic runoff and erosion model: Documentation and user manual. ARS-77. USDA, ARS, Washington, DC.
32. Wösten, J.H.M., A. Lilly,A. Nemes, and C. Le Bas. 1999. Development and use of a database of hydraulic properties of European soils. Geoderma 90:169–185.
33. Wösten, J.H.M., A. Lilly,A. Nemes, and C. Le Bas. 1999. Development and use of a database of hydraulic properties of European soils. Geoderma 90:169–185.