Description of “Sheep” (Subsurface Hydrology Environmental Elementary Processes)

Preface

We disclaim all liability for direct, incidential or consequential damage resulting from the use of this program.

Introduction

All the calculations performed by this program are based either on the MUALEM/ VAN GENUCHTEN (van Genuchten, 1980) model of water retention and unsaturated hydraulic conductivity or on the bimodal water retention and conductivity function of Durner, Priesack and Peters (1994, 2006, 2008). Whenever possible, analytical solutions are used to tackle the so-called ”Elementary Soil Hydrologic Processes” (Kutilek and Nielsen,1994, Bohne, 2005).

This program is not another numerical model to simulate soil water dynamics and no attempt was made to simulate soil water behavior under field conditions.

This description expects users to be familiar with some basic ideas of soil hydrology.

Subject matters of the program

1. Input of VAN GENUCHTEN parameters and saturated soil hydraulic conductivity (van Genuchten, 1980) **:mandatory**
2. Calculation of (2.1) water content, (2.2) differential soil water capacity C, (2.3) unsaturated soil hydraulic conductivity COND, (2.4) relative hydraulic conductivity RELK, (2.5) diffusivity D, and (2.6) dK/dθ from soil water pressure head.
3. Calculations of the same variables as mentioned above from soil water content. For instance, instead of calculation of θ(h) the inverse h(θ) is calculated.
4. Matrix flux potential between two reference pressure values.
5. Steady-state vertical flow from or to groundwater table (numerical solution).
6. Drying of bare soil by evaporation (Gardner, 1959).
7. Internal drainage using groundwater table as bottom boundary condition (Gardner, 1962 Crank, 1975).
8. Unit gradient transient drainage (Sisson et al., 1980).
9. Ponded and disc infiltration (Barry-Haverkamp and Philip equations, Barry et al. 1995)
10. Green and Ampt infiltration (Jury et al., 1991)
11. Midpoint pressure head between irrigation furrows (Lomen and Warrick, 1978).
12. Horizontal one-dimensional steady-state groundwater flow (Busch, Luckner, Tiemer, 1993).
13. Radial symmetric steady-state groundwater flow to or from a well.
14. Steady-state piston flow of a solute considering linear sorption and first-order decay (Jury et al. 1991)
15. Transient solute transport through a soil column (step input) for steady-state water flow (Breakthrough curve, Lapidus and Amundson, 1952).
16. Transient solute transport through a soil column (pulse input) for steady-sate water flow (Jury and Sposito solution, Jury et al., 1991).
17. Two-dimensional horizontal transient solute transport in one-dimensional horizontal steady-state groundwater flow (Csanady solution, Kinzelbach, 1986)

18. Hydrologic total discharge or groundwater recharge estimation (Miegel et al.,2013)
19. Steady-state field drainage (Bodenwasserregulierung, 1985, Skaggs, 1999)
20. Non steady-state field drainage (Storchenegger and Bohne, 2005, Widmoser, 2010)

Using the program

In the beginning, the main menu is written to the screen. First of all, the first menu point must be taken that reads soil hydraulic parameters from the screen or uses default values. Thereafter, you may use the other items as mentioned above. All the results are written to the screen AND to a file. The user is requested to choose the name of that file. This file may be used as an input file for other codes (e.g. gnuplot) to prepare graphs.

The program is written in FORTRAN. As processing of character expressions is rather tedious in this old FORTRAN version, we tried to simplify things somewhat. For that reason you have to type “1” for ”yes” and “0” for ”no”. All the exits throughout the program are exits to the main menu, except the exit in the main menu itself, which terminates the performance of the program. To decide what kind of input is requested in a given situation, it is strongly recommended to read the program output to the screen carefully.

1. Input of soil hydraulic parameters

Measured or PTF-based soil hydraulic parameters may be used to meet parameter requirements.
To obtain parameters from pedotransfer functions, the ANN-based code ROSETTA (Schaap et al., 2001) may be used. Another option is using the pedotransfer function proposed by Zacharias (Zacharias and Wessolek, 2008) or the parameter estimation from grain size distribution after Nimmo et al., 2007. The Vereecken, Zacharias and the Nimmo functions are supported on this website by spreadsheet files.
Still another option is using default values known for soil texture classes of the German soil texture classification (Renger et al., 2009). Furthermore, the data base UNSODA provides a collection of empirical soil data and the code "Twostep", which is part of this website, is suitable to estimate soil hydraulic parameters from observations. The common code to derive soil hydraulic parameters from observations is the program RETC.
A particular feature of the unimodal Mualem-vanGenuchten model of hydraulic conductivity is its steep descend near saturation in case the parameter n is close to its minimum value of 1.05. In this case, the modified formulation of the model (Schaap and van Genuchten, 2006) should be used provided that the same formulation was used beforehand for parameter estimation. This problem is

of less importance when bimodal soil hydraulic functions (Durner, 1994, Priesack and Durner, 2006, Peters and Durner, 2008) are used.

2. Van Genuchten/Mualem model

Water content Θ is calculated from soil water pressure head h according to van Genuchten (1980).

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

$$C=\frac{d\theta}{dh}=\frac{(\theta_s-\theta_r)\,(n-1)\,\alpha^n\,h^{n-1}}{\left(1+(\alpha h)^n\right)^{m+1}} \tag{2}$$

where θ_r, θ_s, α, n are parameters and *h* is the soil water pressure head, taken positive here. In this program, soil water pressure head taken with its correct sign is named h_p. Equation (2) gives the specific water capacity.

To obtain closed-form equations for hydraulic conductivity, the parameter *m* is related to *n* by *m= 1-1/n*. This version of the program is not able to consider any arbitrary m (m>0) not related to *n*.

Following the MUALEM theory, hydraulic conductivity may be calculated by

$$K(S_o(h))=S_o^x\left(\frac{\int_o^{S_o}\frac{1}{h(S)}dS}{\int_o^1\frac{1}{h(S)}dS}\right)^2 \tag{3}$$

K	hydraulic conductivity, cm/d
K_s	saturated soil hydraulic conductivity
h	soil water pressure head, taken positive in unsaturated soil, cm
S	effective saturation, $S=\frac{\theta-\theta_r}{\theta_s-\theta_r}$
x	parameter of tortuosity, recommended value: 0.5
θ	volumetric water content, $cm^3\ cm^{-3}$
s,i,r,0	indices: saturated, initial, residual, reference, respectively

Van Genuchten (1980) developed a closed-form equation of the soil hydraulic conductivity

$$K(h)=K_s\frac{\left[1-(\alpha h)^{n-1}\left(1+(\alpha h)^n\right)^{-m}\right]^2}{\left(1+(\alpha h)^n\right)^{mx}} \tag{4}$$

where m is related to n by $m = 1 - 1/n$

Several researchers found the predicition of hydraulic conductivity to be greatly improved when the matching point is not taken at zero suction, but instead at some different value $h_{p,m}$ of pressure head. Using this option replaces the saturated hydraulic conductivity throughout the program by an apparent value of it which is given by

$$K_{s,app} = \frac{K_{obs}(h_{pm})}{K_{rel,predicted}(h_{pm})}$$

where $K_{obs}(h_{pm})$ is any known value of hydraulic conductivity and $K_{rel,predicted}(h_{pm})$ is the prediction based upon Eq. (4) for K_s=1.

The hydraulic conductivity can be calculated as a function of water content as well:

$$K = K_s S^x \left[1 - \left(1 - S^{1/m}\right)^m\right]^2 \tag{5}$$

Since the diffusivity is defined by $D=K/C$ it is given by

$$D(S) = \frac{K_s S^{x-1/m} \left(\dfrac{1}{A} - 2 + A\right)}{(\theta_s - \theta_r)\,(n-1)\,\alpha} \tag{6}$$

with $$A = \left(1 - S^{1/m}\right)^m \tag{6a}$$

If C is already known it is more convenient to calculate D from $D = K/C$.
Unit gradient methods as mentioned below require knowledge of $dK/d\theta$ which is given by

$$\frac{dK}{d\theta} = \frac{K_s}{\theta_s - \theta_r}\left[2\,PTR\frac{Q}{1-P} + xTR^2\right] \tag{7}$$

with

$$P = S^{1/m};\; T = S^{x-1};\;\; Q = (1-P)^m;\; R = 1 - Q$$

The above mentioned equations are realized in the subroutine VANGEN.

The calculations described are either performed for a single value of h given by input or a list is generated. In the latter case, lower and upper boundaries and the increment have to be specified. The list is written to the screen and to the output file.

3. Inverted van Genuchten relation

This option uses the same equations as mentioned above. Since h is not given by input, it is first calculated from

$$h=\frac{1}{\alpha}\left(\frac{1}{S^{1/m}}-1\right)^{1/n} \tag{10}$$

4. Calculation of matrix flux potential

Matrix flux potential (Kutilek and Nielsen,1994) is defined by

$$\Phi(h_1, h_2) = \int_{h_1}^{h_2} K(h)\,dh \tag{11}$$

This potential is useful to calculate infiltration (Elrick, Reynolds 1992, White et al., 1992). For $h_1 = 0$ it is recommended to use Menu point 9. In the program, Eq. (11) is evaluated numerically using Simpson's procedure.

5. Steady-state vertical flow above groundwater table

The DARCY - equation for vertical steady-state flow is given by

$$q = -K(h_p)\left(\frac{dh_p}{dz} + 1\right) \tag{12}$$

z vertical coordinate, upward positive, z=0 at groundwater table, cm
q flux, cm/d (units must be consistent with z and K), upward positive
h_p soil water pressure head, sign taken correctly.

The separation of variables yields two ordinary differential equations, which can be chosen alternatively. Beginning at the groundwater table, both are solved numerically.

Option 1:

$$dh_p = \left(\frac{q}{K(h_p)} + 1\right) dz \tag{13}$$

Option 2:

$$dz = \frac{1}{\dfrac{q}{K(h_p)} + 1}\, dh_p \tag{14}$$

Equation (13) yields values of pressure head at defined elevations z above groundwater table and equation (14) calculates the elevation z for defined values of h_p .

Use of Equ. (13) requires controlling the increment Δz. Please note that q>0 means upward flow of water while q<0 indicates downward movement. In case of using Equ. (14) a list of q values is generated. For that reason no value of q has to be specified. The numerical procedure continues until a lower threshold value of h_p is reached. To suggest such a value, h_p is first calculated from the midpoint water content between permanent wilting point (h_p=-15800 cm) and water content at h_p= - 63 cm.

The numerical solution of Eq. (13) was compared to an analytical solution, which is available for exponential functions of hydraulic conductivity. No significant deviations were detected.

6. Evaporation from bare soil

Gardner (1959) distinguished two stages of drying bare soils by evaporation. During the first stage, evaporation depends on external atmospheric conditions. In the second stage, real evaporation depends no longer on external conditions but on flow conditions in soil. In this stage, the water content at the soil surface θ_0 remains constant and the flux q_0 from inner soil to the soil surface decreases with time, *t*. As long as the initial water content at the lower boundary is maintained, the flux to the soil surface is given by

$$q(t)=\left(\theta_i-\theta_0\right)\sqrt{\frac{D(\theta_0)}{\pi t}} \tag{15}$$

Integration of Eq.(15) yields the cumulative amount of evaporation

$$E(t)=2\left(\theta_i-\theta_0\right)\sqrt{\frac{D(\theta_0)t}{\pi}} \tag{16}$$

Since θ_0 is constant, *D* is constant as well.

7. Internal drainage

In the first step, this option calculates the water storage *W* (unit cm) of a soil profile in equilibrium with groundwater table. The term “equilibrium” denotes a condition of zero flux anywhere in the soil profile. Water storage in a soil column of length *L* (that means that *L* represents the groundwater depth) is then given by

$$W_\infty=\int_o^L \theta\left(h_p(z)\right)\,dz \tag{17}$$

The integration is done numerically by Simpson’s procedure.

In the second step, the program calculates non-steady-state internal drainage. At time t=0 the soil profile is assumed to be (almost) saturated. Under field conditions, a certain amount of entrapped air is always present. On top of the soil column a flux boundary condition is assumed, given by

$q = 0$. The groundwater table represents the bottom of the soil column. Internal drainage is calculated by an iteration procedure for a given drainage time t (days).
The amount of water drained from the soil profile in infinite time is given by

$$Q_\infty = \theta_s L - W_\infty \tag{18}$$

This equation indicates that Q is of the same unit as W or L. If we denote the amount of water drained from the soil profile during drainage time t by Q_t we may use the fraction Q_t / Q_∞ as an indicator of the drainage ratio.
To estimate Q_t , the analytical solution to the flow equation given by Gardner (1962) is used. His solution reads

$$Q_t = Q_\infty \left[1 - \sum_{j=0}^{j=3} \left(\frac{1}{\pi^2 (2j+1)^2} \exp\left(- \frac{D_c (2j+1) \pi^2 t}{4L^2} \right) \right) \right] \tag{19}$$

Mathematically, the upper limit of the sum should be infinite and not merely “3”. Since the value of the series converges rapidly, consideration of 4 terms will do. The equation holds for constant diffusivity D only. To correct for variable D an iterative procedure is used. Eq.(19) is calculated for an effective constant D_c that is best represented by the mean according to CRANK (1975)

$$D_C = \frac{1.85}{\left(\theta_i - \theta_f\right)^{1.85}} \int D(\theta) \left(\theta_i - \theta_f\right)^{0.85} d\theta \tag{20}$$

For integration, again SIMPSON’s rule is used. In this equation is θ_i the initial soil water content which is assumed to be near saturation. θ_f represents the final water content, which is unknown in the beginning. To calculate D from Eq. (6), in the first step of iteration complete drainage during the time chosen is assumed and approximated by $h_p = - L/2$. After calculation of Q_t, the improved final water content is given by

$$\theta_f = \theta_i - Q_t / L$$

In the following iteration steps the results from the previous steps are used. The procedure is terminated when the difference between estimated and calculated final water content values is very small.

8. Unit gradient transient drainage

Internal drainage of a very long soil column (or a very deep groundwater table, respectively) continues for a very long period of time and only seldom this will be of interest. Most users are interested in soil water storage of a soil profile of limited depth. In soil profiles over a deep groundwater table the bottom boundary condition may be approximated by the unit-gradient assumption. That is, the hydraulic gradient is assumed to be unity. Numerical experiments have shown this assumption to be reliable for depths between 1 and 2 m and for drainage times between t=1 and t=100 days. SISSON et al. (1980) developed the analytical solution

$$\frac{dK}{d\theta}=\frac{z}{t} \qquad (21)$$

For the left-hand side, Eq. (7) is used. Since there is no way to solve the resulting equation for θ explicitly, an implicit solution has to be used, which is performed by the procedure NEWTON. Water content values of soil compartments (thickness 1 cm) are then integrated by means of the SIMPSON subroutine to give the water storage between the soil surface and the required depth.

9. Infiltration

Preparations

In this section of the program, at first the matrix flux potential is calculated, which is defined by

$$\Phi=\int_{h_0}^{h_i} K(h)\,dh \qquad (22)$$

h_o Soil water pressure head at the infiltrating surface

h_i Initial soil water pressure head prior to infiltration.

To solve the integral, we felt it appropriate to use a stepwise analytical solution rather than the SIMPSON procedure. For exponential hydraulic conductivity, Gardner proposed

$$K(h)=K_s\exp(-\alpha h) \qquad (23)$$

Please note that h>0 is used here. The analytical solution to Eq. (22) using Eq.(23) is given by

$$\Phi_{hb}^{ht}=\frac{K_s}{\alpha}\exp\left(\alpha\left(h_t-h_b\right)\right) \qquad (24)$$

h_t — h at top of an interval
h_b — h at bottom of an interval
h_m — h at mid-point of the interval

For the purpose of integration the x-axis is subdivided into N intervals, each having a different α_j Substituting (23) into (22) and summing over all *j*'s, leads to the following numerical approximation for the matric flux potential

$$\Phi=\sum_{j=1}^{N}\frac{K_s}{\alpha_j}\left(\exp(\alpha_j h_{j+1/2}-\exp(\alpha_j h_{j-1/2})\right)$$

The conductivity function (23) can be expressed in terms of the vanGenuchten/Mualem parameters by using suitable expressions for α_j. Equating the two conductivity expressions at the midpoint h_m of each interval yields

$$\alpha=\frac{1}{h_m}\ln\left(\frac{K(h_m)}{K_s}\right)$$

where $K(h_m)$ is the hydraulic conductivity according to Eq. 4 (or 8, resp.), evaluated at

$$h_m=\frac{1}{2}\left(h_{j-1/2}+h_{j+1/2}\right)$$

To account for hysteresis approximately, the parameter α may be doubled (Luckner et al., 1989). Next, sorptivity (Philip, 1987, Jury et al., 1991, White et al., 1992) is obtained from

$$S_0=\sqrt{1.82\ \Delta\theta\ \Phi} \qquad (25)$$

where $\Delta\theta=\theta(h_0)-\theta(h_i)$

One-dimensional vertical infiltration

In case of ponded infiltration, the final water content is assumed to be $0.95\theta_S$. The constant 0.95 is an empirical value to account for entrapped air. Now the truncated infiltration formula after Philip (1987, see Jury et al., 1991) can be applied yielding the cumulative infiltration

$$I=S_0\sqrt{t}+At \qquad (26)$$

One of the problems inherent in the truncated equation consists in the time-dependent relationship between A and the hydraulic conductivity $K(h_0)$ at top of the soil profile. The computer code described here assumes $A = 0.6\ K(h_0)$.

BARRY, HAVERKAMP et al. (1995) have proposed an infiltration equation containing only parameters, which are not time-dependent and retain a sound physical meaning. The explicit form of this equation is given by Eq. 27:

$$I = 1 + T - \gamma \exp\left[\frac{-\sqrt{2T}}{1+\sqrt{2T}/6} - \frac{2T}{3}\right] + \frac{\gamma}{1+T}\exp\left(\frac{-2T}{3}\right)\left[1-(1-\gamma)^{8} T^{5/2}\right] + (2\gamma + T)\ln(1+T/\gamma)$$

In this equation, the capital letters I and T indicate dimensionless variables. The relationships between dimensionless and dimensioned variables are given by

$$I = (q_i - K_i t)\frac{2(K_0 - K_i)}{S_0^2 + 2K_0 h_{surf} \Delta\theta}$$

$$T = \frac{2t(K_0 - K_i)^2}{S_0{}^2 + 2K_0 h_{surf} \Delta\theta} \quad (28)$$

q_i	infiltration rate
h_{surf}	height of water column ponded on the soil surface
h_{str}	air-entry point on the wetting branch of the water retention curve
t	infiltration time
K_s	saturated soil hydraulic conductivity
index i	initial value (prior to infiltration)
index 0	value at the infiltrating surface

$$\Delta\theta = \theta(h_0) - \theta(h_i)\ ;\ K_0 = K(h_0)\ ;\ K_i = K(h_i)$$

The term γ represents the expression

$$\gamma = \frac{2K_0(h_{surf} - h_{str})\Delta\theta}{S^2 + 2K_0 h_{surf}\Delta\theta} \quad (29)$$

and should range between 0 and 1.

The parameter h_{str} is not an independent soil parameter. According to FUENTES et al. (1992), it can be approximated by

$$\lambda_s = \frac{1}{K_0}\int_{-\infty}^{h_0}\left(2\frac{K(h) - K_i}{(K_0 - K_i)S_e(h)} - 1\right)K(h)\,dh \quad (30)$$

and

$$h_{str} = \lambda_s \frac{K_0 - K_i}{K_0} \quad (31)$$

S_e effective saturation (or relative water content, *RWC*)

To apply these equations, first γ and h_{str} are calculated because they do not depend on infiltration time. Again the procedure of SIMPSON is used to integrate Eq.(29).

FUENTES derived from his theory restrictions concerning the value of VAN-GENUCHTEN-parameters. If these restrictions are not met, the values of γ and h_{str} are outside their permitted boundaries and default standard assumptions apply. The parameter h_{str} is said to be rather insensitive.

Three-dimensional infiltration from a disc infiltrometer

Smettem et al.(1994) developed an approximate solution to infiltration from the disc of a tension infiltrometer. Their equation reads

$$i_{3D} = i_{1D} + 0.75\pi\, r \frac{S_0{}^2 t}{\Delta\theta} \qquad (31a)$$

- r radius of the disc, cm
- i_{3D} three-dimensional cumulative volume of infiltrated water, cm^3
- i_{1D} one-dimensional cumulative volume of infiltrated water, cm^3
- S_0 sorptivity, (cm time $^{-0.5}$)
- t time

In this case, h_0 will be in general different from zero.

10. Green & Ampt infiltration

From many applications it is known, that the Green & Ampt infiltration equation yields disappointing results (Kutilek, Nielsen 1994). However, comparisons between the Green&Ampt method and results of the numerical model HYDRUS 1D have shown sufficient agreement for sandy and loamy soils over shallow groundwater table. We recommend using an empirical soil water pressure head h_0 to calculate the initial soil water content $\theta(h_0)$ and to evaluate the pressure head at the wetting front h_F from

$$h_F = \frac{1}{K_s} \int_0^{h_0} K(h)\, dh \qquad (32)$$

(Kutilek, Nielsen 1994, Neumann's formula). Recommended values of h_0 are given by:

Texture Class (U.S. Soil Conservation Service)	**h_0 cm**
Sand	11
Loamy Sand	14
Sandy Loam	29
Sandy Clay Loam	45
Loam	55
Clay Loam	58

The Green&Ampt infiltration is given by

$$t(L)=\frac{\Delta\theta}{K_s}\left[L-h_F\ln\frac{L+h_F}{h_F}\right]\quad;\quad I=L\Delta\theta \tag{33}$$

t		time, days
K_s		saturated soil hydraulic conductivity, cm/day
L		depth of the wetting front, cm
$\Delta\theta$	=	$\theta_s-\theta(h_0)$
I		cumulative infiltration, cm

11. Soil moisture under furrow irrigation

Furrow irrigation is a process involving simultaneous non-steady state flow of water in furrows and two-dimensional infiltration into soil. Irrigation systems should be designed to provide access to water for plant roots everywhere between irrigation furrows and to avoid large losses of water due to drainage.

Important parameters of a furrow irrigation system are:

- Spacing of furrows, L (cm),
- source strength Q (Liters per day and per meter furrow length),
- depth of root water uptake z_0 , cm,
- length of furrows (not considered here), and
- daily evapotranspiration u, cm/d

To give only a first crude approximation, a method developed by Lomen and Warrick (1978, Warrick et al. 1979) is used here to calculate soil water pressure head near the soil surface at the midpoint between furrows. Since all the analytical solutions used here are based upon Gardner's exponential conductivity function (Eq. 23), we first have to adjust the Gardner hydraulic conductivity to the Mualem/ vanGenuchten soil hydraulic conductivity. The simplest way to do this is to match both at a selected value h_{match}. The computer code uses h = 60 cm as matching point. This yields for Gardner's α

$$\alpha=-\frac{1}{h_{match}}\ln\left(\frac{K(h_{match})}{K_s}\right)$$

The midpoint soil water pressure (cm) is given by

$$h_M=\frac{1}{\alpha}\ln\left\{\frac{Q}{K_s L}\left[\exp(-0.24\,\alpha L)+\frac{r_u}{\alpha z_0}\left(\exp(\alpha z_0)-1\right)\right]\right\} \tag{34}$$

r_u represents the fraction of evapotranspiration relative to total water supply (mm/mm).